



# Full wwPDB/EMDataBank EM Map/Model Validation Report ⓘ

Apr 12, 2017 – 09:41 PM EDT

PDB ID : 5FKU  
EMDB ID: : EMD-3201  
Title : cryo-EM structure of the E. coli replicative DNA polymerase complex in DNA free state (DNA polymerase III alpha, beta, epsilon, tau complex)  
Authors : Fernandez-Leiro, R.; Conrad, J.; Scheres, S.H.W.; Lamers, M.H.  
Deposited on : 2015-10-20  
Resolution : 8.34 Å(reported)

This is a Full wwPDB/EMDataBank EM Map/Model Validation Report  
for a publicly released PDB/EMDB 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/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20029077

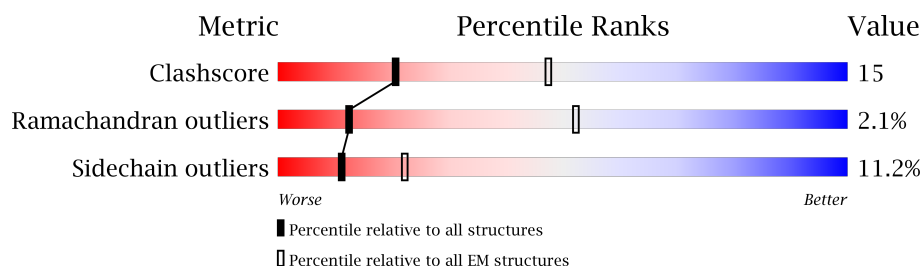
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 8.34 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)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	1160	
2	B	366	
2	C	366	
3	D	243	
4	E	144	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17387 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 POLYMERASE III SUBUNIT ALPHA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1149	Total	C	N	O	S	0	0
			9050	5738	1567	1697	48		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	921	LEU	ALA	ENGINEERED MUTATION	UNP P10443
A	923	LEU	MET	ENGINEERED MUTATION	UNP P10443

- Molecule 2 is a protein called DNA POLYMERASE III SUBUNIT BETA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	366	Total	C	N	O	S	0	0
			2844	1786	498	541	19		
2	C	366	Total	C	N	O	S	0	0
			2844	1786	498	541	19		

- Molecule 3 is a protein called DNA POLYMERASE III SUBUNIT EPSILON.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	218	Total	C	N	O	S	0	0
			1709	1085	298	318	8		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	183	LEU	THR	ENGINEERED MUTATION	UNP P03007
D	185	LEU	MET	ENGINEERED MUTATION	UNP P03007
D	186	PRO	ALA	ENGINEERED MUTATION	UNP P03007
D	187	LEU	PHE	ENGINEERED MUTATION	UNP P03007

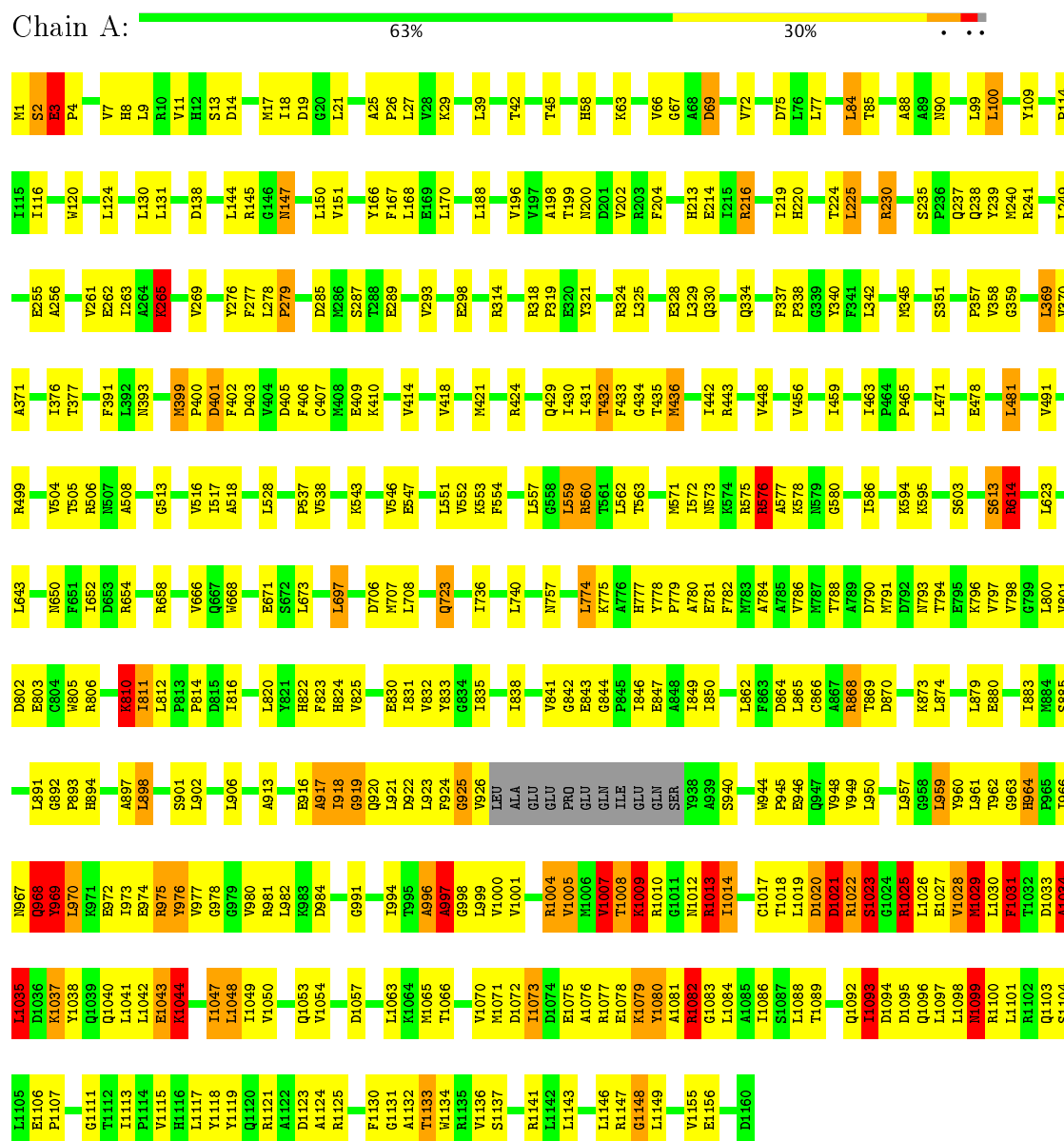
- Molecule 4 is a protein called DNA POLYMERASE III SUBUNIT TAU.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	120	Total	C	N	O	S	0	0
			940	582	170	186	2		

### 3 Residue-property plots

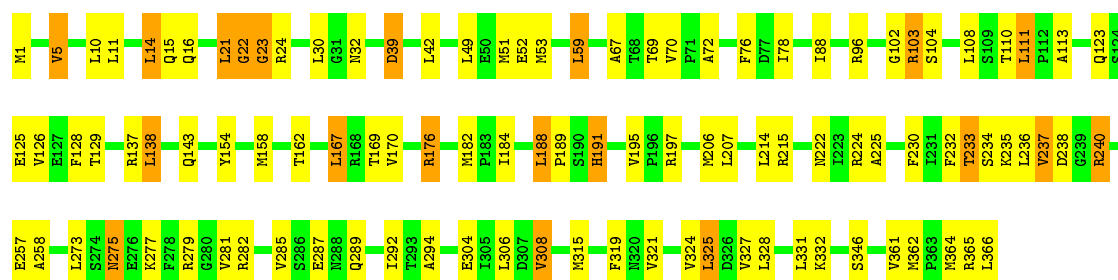
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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. 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 POLYMERASE III SUBUNIT ALPHA



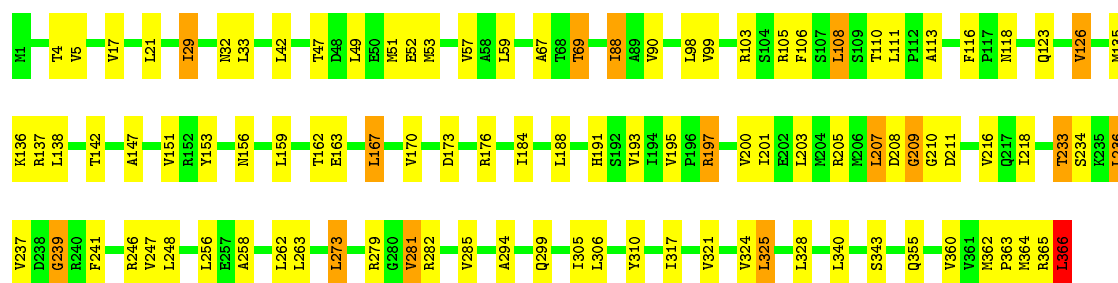
#### • Molecule 2: DNA POLYMERASE III SUBUNIT BETA





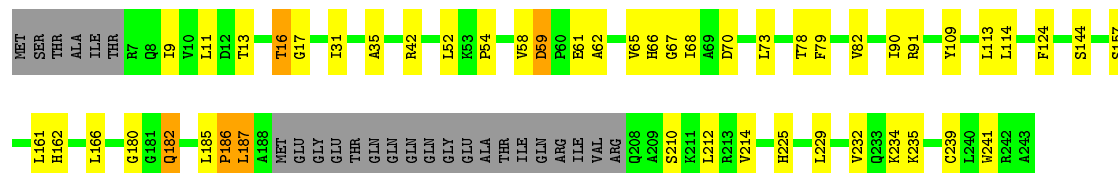
• Molecule 2: DNA POLYMERASE III SUBUNIT BETA

Chain C: 72% 23% .



• Molecule 3: DNA POLYMERASE III SUBUNIT EPSILON

Chain D: 70% 18% 10% .



• Molecule 4: DNA POLYMERASE III SUBUNIT TAU

Chain E: 57% 22% 17% .



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	16970	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	each particle	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	28409	Depositor
Image detector	GATAN K2 QUANTUM (4K X 4K)	Depositor

## 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  >2	RMSZ	# Z  >2
1	A	0.54	1/9230 (0.0%)	0.90	24/12470 (0.2%)
2	B	0.50	0/2893	0.89	4/3915 (0.1%)
2	C	0.51	0/2893	0.90	3/3915 (0.1%)
3	D	0.48	0/1739	0.72	0/2348
4	E	0.54	0/953	0.81	2/1293 (0.2%)
All	All	0.52	1/17708 (0.0%)	0.88	33/23941 (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
1	A	0	20
2	B	0	1
3	D	0	4
4	E	0	1
All	All	0	26

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1082	ARG	CD-NE	5.41	1.55	1.46

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1043	GLU	C-N-CA	-13.09	88.99	121.70
1	A	278	LEU	C-N-CD	-10.16	98.25	120.60
1	A	1082	ARG	NE-CZ-NH1	10.12	125.36	120.30
1	A	1044	LYS	N-CA-C	9.00	135.29	111.00
1	A	1043	GLU	CA-C-N	8.41	135.69	117.20
1	A	1043	GLU	O-C-N	-7.33	110.97	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1082	ARG	CD-NE-CZ	6.82	133.15	123.60
1	A	1043	GLU	N-CA-C	6.73	129.18	111.00
1	A	614	ARG	NE-CZ-NH1	6.72	123.66	120.30
2	B	365	ARG	NE-CZ-NH1	6.65	123.63	120.30
1	A	975	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	A	560	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	A	265	LYS	CD-CE-NZ	5.95	125.39	111.70
2	B	197	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	A	1023	SER	N-CA-C	5.85	126.79	111.00
4	E	615	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	A	337	PHE	N-CA-C	5.73	126.47	111.00
2	C	239	GLY	N-CA-C	5.69	127.31	113.10
1	A	970	LEU	N-CA-C	5.68	126.33	111.00
1	A	230	ARG	NE-CZ-NH1	5.62	123.11	120.30
4	E	615	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	A	898	LEU	CB-CG-CD2	5.48	120.32	111.00
1	A	997	ALA	N-CA-CB	-5.39	102.56	110.10
1	A	1093	ILE	O-C-N	-5.28	114.25	122.70
1	A	225	LEU	CA-CB-CG	5.26	127.41	115.30
1	A	1013	ARG	NE-CZ-NH1	5.22	122.91	120.30
2	B	23	GLY	N-CA-C	5.20	126.10	113.10
1	A	1082	ARG	N-CA-C	-5.17	97.04	111.00
1	A	1025	ARG	NE-CZ-NH1	5.15	122.87	120.30
2	C	366	LEU	CA-CB-CG	5.12	127.07	115.30
2	B	39	ASP	CB-CA-C	5.10	120.60	110.40
2	C	209	GLY	N-CA-C	5.06	125.76	113.10
1	A	969	TYR	N-CA-C	5.06	124.65	111.00

There are no chirality outliers.

All (26) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1001	VAL	Peptide
1	A	1021	ASP	Peptide
1	A	1028	VAL	Peptide
1	A	1029	MET	Peptide
1	A	1031	PHE	Peptide
1	A	1033	ASP	Peptide
1	A	1034	ALA	Peptide
1	A	1047	ILE	Peptide
1	A	1093	ILE	Mainchain,Peptide
1	A	1099	ASN	Mainchain

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Mol	Chain	Res	Type	Group
1	A	2	SER	Peptide
1	A	279	PRO	Mainchain
1	A	3	GLU	Peptide
1	A	465	PRO	Peptide
1	A	576	ARG	Mainchain
1	A	917	ALA	Peptide
1	A	919	GLY	Peptide
1	A	969	TYR	Mainchain
1	A	996	ALA	Peptide
2	B	21	LEU	Peptide
3	D	185	LEU	Peptide
3	D	186	PRO	Peptide
3	D	187	LEU	Peptide
3	D	67	GLY	Mainchain
4	E	533	PRO	Mainchain

## 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	9050	0	9006	402	0
2	B	2844	0	2861	47	0
2	C	2844	0	2861	51	0
3	D	1709	0	1706	27	0
4	E	940	0	940	23	0
All	All	17387	0	17374	528	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 15.

All (528) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1040:GLN:O	1:A:1043:GLU:HG2	1.25	1.30
1:A:1040:GLN:HG3	1:A:1043:GLU:OE2	1.28	1.28
1:A:775:LYS:O	1:A:779:PRO:HG3	1.29	1.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1078:GLU:HA	1:A:1082:ARG:NH1	1.66	1.11
1:A:775:LYS:O	1:A:779:PRO:CG	2.02	1.07
1:A:924:PHE:HB2	1:A:925:GLY:HA3	1.37	1.06
1:A:1028:VAL:HG23	1:A:1029:MET:HB2	1.38	1.06
1:A:1013:ARG:CG	1:A:1014:ILE:HG22	1.87	1.04
4:E:505:LYS:O	4:E:506:THR:OG1	1.74	1.04
1:A:1040:GLN:HG3	1:A:1043:GLU:CD	1.81	1.01
1:A:1040:GLN:CG	1:A:1043:GLU:OE2	2.13	0.95
1:A:963:GLY:C	1:A:967:ASN:OD1	2.06	0.93
1:A:924:PHE:HB2	1:A:925:GLY:CA	2.00	0.92
1:A:1040:GLN:O	1:A:1043:GLU:CG	2.18	0.91
1:A:1072:ASP:O	1:A:1076:ALA:N	2.04	0.90
3:D:11:LEU:HD13	3:D:35:ALA:HB2	1.54	0.89
1:A:1043:GLU:HB2	1:A:1044:LYS:HG3	1.56	0.86
1:A:1072:ASP:N	1:A:1075:GLU:HB3	1.90	0.86
1:A:1013:ARG:HG3	1:A:1014:ILE:HG22	1.57	0.86
1:A:1043:GLU:CB	1:A:1044:LYS:HG3	2.06	0.86
1:A:1048:LEU:HD11	1:A:1050:VAL:HG13	1.57	0.86
1:A:810:LYS:HA	1:A:811:ILE:O	1.76	0.85
1:A:1028:VAL:HA	1:A:1029:MET:CB	2.07	0.85
1:A:869:THR:HG21	1:A:874:LEU:HD12	1.59	0.84
1:A:1013:ARG:HG2	1:A:1014:ILE:HG22	1.57	0.84
1:A:924:PHE:CB	1:A:925:GLY:HA3	2.07	0.83
1:A:1082:ARG:N	1:A:1082:ARG:HD3	1.94	0.83
1:A:623:LEU:HD13	1:A:652:ILE:HG12	1.61	0.82
1:A:961:LEU:O	1:A:962:THR:OG1	1.97	0.82
2:C:32:ASN:HB3	2:C:69:THR:HG23	1.61	0.82
1:A:802:ASP:OD1	1:A:1022:ARG:HB2	1.81	0.81
1:A:1020:ASP:HA	1:A:1021:ASP:O	1.79	0.81
1:A:1028:VAL:CG2	1:A:1029:MET:HB2	2.09	0.81
1:A:77:LEU:HD21	1:A:150:LEU:HD21	1.63	0.81
1:A:431:ILE:HD11	1:A:508:ALA:HB1	1.63	0.80
1:A:811:ILE:C	1:A:812:LEU:HD22	2.01	0.80
1:A:1008:THR:O	1:A:1009:LYS:HG2	1.82	0.80
1:A:1028:VAL:HA	1:A:1029:MET:CG	2.14	0.78
3:D:16:THR:HG22	3:D:58:VAL:HA	1.64	0.77
1:A:778:TYR:HB3	1:A:781:GLU:OE1	1.85	0.77
1:A:1076:ALA:O	1:A:1079:LYS:CB	2.33	0.77
1:A:198:ALA:HB2	1:A:256:ALA:HB1	1.67	0.77
1:A:1034:ALA:HB2	1:A:1038:TYR:CD1	2.20	0.76
3:D:16:THR:HG23	3:D:31:ILE:CG2	2.16	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:16:THR:HG23	3:D:31:ILE:HG21	1.66	0.76
1:A:1034:ALA:HB2	1:A:1038:TYR:CG	2.21	0.75
1:A:167:PHE:CE2	1:A:263:ILE:HD11	2.20	0.75
2:B:30:LEU:HD11	2:B:49:LEU:HD13	1.67	0.75
1:A:960:TYR:CD2	1:A:964:HIS:CE1	2.75	0.75
1:A:964:HIS:N	1:A:967:ASN:HB3	2.01	0.74
2:C:317:ILE:HD12	2:C:343:SER:HA	1.70	0.74
1:A:975:ARG:O	1:A:977:VAL:HG23	1.88	0.73
1:A:1078:GLU:HA	1:A:1082:ARG:HH11	1.49	0.72
1:A:1076:ALA:O	1:A:1079:LYS:HB2	1.89	0.72
1:A:923:LEU:HD23	2:C:362:MET:HG3	1.70	0.72
1:A:1050:VAL:HG12	1:A:1070:VAL:HA	1.71	0.71
1:A:1028:VAL:HG11	1:A:1065:MET:O	1.90	0.71
1:A:1094:ASP:HA	1:A:1097:LEU:HD13	1.72	0.71
1:A:805:TRP:CH2	1:A:811:ILE:HG21	2.25	0.71
1:A:1038:TYR:O	1:A:1042:LEU:HG	1.90	0.71
1:A:1104:SER:OG	1:A:1147:ARG:NH1	2.25	0.70
1:A:978:GLY:O	1:A:982:LEU:HG	1.92	0.69
1:A:810:LYS:CA	1:A:811:ILE:HB	2.21	0.69
1:A:1007:VAL:O	1:A:1008:THR:HG22	1.92	0.69
1:A:1123:ASP:OD2	4:E:614:ALA:HB3	1.92	0.69
2:B:176:ARG:HB3	2:B:361:VAL:HG12	1.74	0.69
1:A:1082:ARG:H	1:A:1082:ARG:HD3	1.57	0.69
1:A:913:ALA:O	1:A:916:GLU:HB3	1.93	0.69
1:A:614:ARG:HG2	1:A:614:ARG:HH11	1.56	0.69
4:E:616:GLU:O	4:E:619:ILE:HG22	1.93	0.68
2:C:281:VAL:HG23	2:C:294:ALA:HB2	1.75	0.68
1:A:811:ILE:O	1:A:812:LEU:HD22	1.93	0.68
1:A:964:HIS:H	1:A:967:ASN:HB3	1.58	0.67
4:E:524:ALA:HB2	4:E:599:PRO:HB3	1.76	0.67
1:A:1123:ASP:OD2	4:E:614:ALA:CB	2.43	0.67
1:A:944:TRP:CD1	1:A:948:VAL:HG23	2.30	0.67
1:A:810:LYS:N	1:A:811:ILE:HB	2.10	0.66
1:A:963:GLY:HA3	1:A:967:ASN:CG	2.16	0.66
1:A:400:PRO:O	1:A:402:PHE:N	2.28	0.66
1:A:573:ASN:O	1:A:576:ARG:HB3	1.96	0.65
2:B:32:ASN:HB3	2:B:69:THR:HG22	1.79	0.65
1:A:3:GLU:H	1:A:4:PRO:HD3	1.60	0.65
1:A:784:ALA:O	1:A:788:THR:HG23	1.96	0.65
1:A:1043:GLU:HB2	1:A:1044:LYS:CG	2.26	0.65
1:A:1072:ASP:H	1:A:1075:GLU:HB3	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1072:ASP:H	1:A:1075:GLU:CB	2.10	0.64
1:A:791:MET:SD	1:A:822:HIS:NE2	2.71	0.64
2:C:126:VAL:HG11	2:C:191:HIS:HB3	1.80	0.64
1:A:1028:VAL:HA	1:A:1029:MET:HB2	1.80	0.64
4:E:554:LEU:HD12	4:E:586:LEU:HD11	1.79	0.63
4:E:606:ILE:O	4:E:609:GLU:HG3	1.99	0.63
1:A:968:GLN:HG2	1:A:969:TYR:CZ	2.33	0.63
1:A:471:LEU:HD13	1:A:499:ARG:HG3	1.81	0.63
1:A:1005:VAL:HG23	1:A:1014:ILE:HG21	1.81	0.63
1:A:1136:VAL:HG12	1:A:1137:SER:O	2.00	0.62
2:B:16:GLN:NE2	2:B:206:MET:HA	2.14	0.62
1:A:1130:PHE:CE2	1:A:1132:ALA:HB3	2.34	0.62
2:B:281:VAL:HG22	2:B:294:ALA:HB2	1.80	0.62
1:A:833:TYR:CE2	1:A:957:LEU:HD13	2.35	0.62
1:A:923:LEU:HD23	2:C:362:MET:CG	2.29	0.62
1:A:843:GLU:O	1:A:846:ILE:HG12	1.99	0.62
1:A:1012:ASN:O	1:A:1013:ARG:NE	2.31	0.62
1:A:775:LYS:O	1:A:779:PRO:CD	2.47	0.62
1:A:1071:MET:HB2	1:A:1075:GLU:HG2	1.81	0.61
1:A:1048:LEU:HD11	1:A:1050:VAL:CG1	2.29	0.61
1:A:1048:LEU:HD21	1:A:1050:VAL:HG13	1.83	0.61
1:A:358:VAL:O	1:A:562:LEU:HG	2.01	0.61
1:A:977:VAL:HG12	1:A:980:VAL:HG13	1.81	0.61
1:A:794:THR:O	1:A:798:VAL:HG23	2.00	0.61
2:B:279:ARG:HB3	2:B:321:VAL:HG12	1.82	0.61
1:A:1048:LEU:CD1	1:A:1050:VAL:HG13	2.30	0.61
1:A:1093:ILE:CG1	1:A:1096:GLN:H	2.14	0.61
1:A:429:GLN:HB2	1:A:538:VAL:HG12	1.83	0.60
1:A:810:LYS:O	1:A:830:GLU:HB3	2.01	0.60
1:A:960:TYR:HD2	1:A:964:HIS:CE1	2.17	0.60
1:A:673:LEU:HD21	1:A:697:LEU:HD23	1.83	0.60
1:A:975:ARG:O	1:A:976:TYR:HD1	1.84	0.60
1:A:1040:GLN:C	1:A:1043:GLU:HG2	2.17	0.60
1:A:340:TYR:CE1	1:A:552:VAL:HG11	2.37	0.60
2:C:159:LEU:HD13	2:C:241:PHE:HB3	1.84	0.60
2:B:346:SER:OG	2:B:362:MET:SD	2.60	0.60
1:A:430:ILE:HD11	1:A:516:VAL:HB	1.83	0.59
1:A:409:GLU:OE2	1:A:563:THR:OG1	2.20	0.59
1:A:1076:ALA:O	1:A:1079:LYS:HB3	2.02	0.59
1:A:459:ILE:HD13	1:A:491:VAL:HG22	1.85	0.59
1:A:1072:ASP:N	1:A:1075:GLU:CB	2.63	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:798:VAL:O	1:A:801:VAL:HG22	2.02	0.59
1:A:168:LEU:HB2	1:A:196:VAL:HG12	1.85	0.59
1:A:802:ASP:OD1	1:A:1022:ARG:CB	2.50	0.59
1:A:1071:MET:HE2	1:A:1075:GLU:O	2.03	0.59
1:A:1093:ILE:CD1	1:A:1095:ASP:HB2	2.34	0.58
1:A:968:GLN:HG2	1:A:969:TYR:CE2	2.39	0.58
1:A:1103:GLN:O	1:A:1107:PRO:HD2	2.03	0.58
1:A:816:ILE:HG23	1:A:849:ILE:HG23	1.85	0.58
1:A:613:SER:OG	1:A:984:ASP:OD2	2.20	0.58
1:A:996:ALA:HB2	1:A:1049:ILE:HG12	1.85	0.58
1:A:471:LEU:HD13	1:A:499:ARG:CG	2.34	0.58
2:C:4:THR:HG23	2:C:88:ILE:O	2.03	0.58
1:A:1043:GLU:C	1:A:1044:LYS:HG3	2.24	0.57
1:A:3:GLU:N	1:A:4:PRO:HD3	2.17	0.57
4:E:530:LEU:HD13	4:E:575:ALA:HB1	1.85	0.57
1:A:1083:GLY:HA2	1:A:1156:GLU:OE1	2.04	0.57
1:A:880:GLU:O	1:A:883:ILE:HG22	2.03	0.57
1:A:1043:GLU:CG	1:A:1044:LYS:HG3	2.34	0.57
1:A:1078:GLU:CA	1:A:1082:ARG:NH1	2.55	0.57
1:A:1121:ARG:HB3	1:A:1124:ALA:O	2.04	0.57
2:B:162:THR:HG22	2:B:167:LEU:HG	1.86	0.57
1:A:1078:GLU:O	1:A:1079:LYS:C	2.41	0.57
1:A:879:LEU:HD11	1:A:906:LEU:HD21	1.87	0.57
1:A:167:PHE:CD2	1:A:263:ILE:HD11	2.39	0.57
1:A:1034:ALA:CB	1:A:1038:TYR:HB2	2.35	0.56
1:A:276:TYR:HE2	1:A:399:MET:HG3	1.71	0.56
1:A:862:LEU:HD11	1:A:902:LEU:CD2	2.36	0.56
1:A:325:LEU:HD12	1:A:370:VAL:HG22	1.87	0.56
1:A:559:LEU:HD13	1:A:560:ARG:H	1.69	0.56
1:A:314:ARG:O	1:A:318:ARG:HB2	2.05	0.56
4:E:576:LEU:HD12	4:E:586:LEU:HD22	1.87	0.56
1:A:400:PRO:C	1:A:402:PHE:H	2.05	0.56
1:A:902:LEU:O	1:A:906:LEU:HG	2.05	0.56
4:E:505:LYS:HD2	4:E:506:THR:HG23	1.87	0.56
1:A:697:LEU:HD22	1:A:736:ILE:HD13	1.85	0.56
1:A:72:VAL:HG22	1:A:116:ILE:HD11	1.87	0.56
1:A:963:GLY:HA3	1:A:967:ASN:ND2	2.20	0.56
1:A:923:LEU:HD22	2:C:247:VAL:CG1	2.36	0.56
1:A:1028:VAL:CA	1:A:1029:MET:CB	2.83	0.56
1:A:1012:ASN:O	1:A:1013:ARG:HB3	2.06	0.55
1:A:782:PHE:O	1:A:786:VAL:HG23	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:966:ILE:C	1:A:968:GLN:HE22	2.09	0.55
2:C:29:ILE:HG23	2:C:111:LEU:HD23	1.88	0.55
1:A:1034:ALA:CB	1:A:1038:TYR:CD1	2.88	0.55
1:A:1143:LEU:O	1:A:1146:LEU:HB3	2.06	0.55
1:A:924:PHE:CD2	1:A:925:GLY:HA3	2.40	0.55
1:A:431:ILE:HD11	1:A:508:ALA:CB	2.36	0.55
1:A:1034:ALA:O	1:A:1035:LEU:HD12	2.07	0.55
1:A:442:ILE:HD12	1:A:463:ILE:HG13	1.88	0.55
3:D:161:LEU:O	3:D:166:LEU:HD22	2.07	0.55
1:A:357:PRO:HB3	1:A:562:LEU:HB3	1.89	0.55
1:A:963:GLY:O	1:A:967:ASN:OD1	2.24	0.55
3:D:180:GLY:O	3:D:182:GLN:N	2.40	0.55
1:A:478:GLU:HB3	1:A:481:LEU:HD22	1.88	0.55
1:A:944:TRP:NE1	1:A:948:VAL:HG23	2.22	0.55
3:D:16:THR:HG22	3:D:58:VAL:HG22	1.87	0.55
1:A:84:LEU:HD23	1:A:131:LEU:O	2.07	0.55
1:A:255:GLU:HG3	3:D:214:VAL:HG22	1.88	0.55
1:A:1148:GLY:C	1:A:1149:LEU:HD12	2.28	0.54
1:A:1034:ALA:HB3	1:A:1038:TYR:HB2	1.88	0.54
1:A:964:HIS:N	1:A:967:ASN:CB	2.70	0.54
1:A:963:GLY:C	1:A:967:ASN:CG	2.66	0.54
1:A:576:ARG:HG3	1:A:577:ALA:N	2.22	0.54
2:B:5:VAL:HG13	2:B:59:LEU:HD12	1.88	0.54
1:A:85:THR:HB	1:A:131:LEU:HD12	1.90	0.54
2:C:285:VAL:HG22	2:C:310:TYR:CD2	2.42	0.54
2:C:33:LEU:O	2:C:69:THR:HA	2.07	0.54
1:A:803:GLU:O	1:A:806:ARG:HG2	2.08	0.54
2:C:321:VAL:HG22	2:C:325:LEU:HD22	1.90	0.54
1:A:1079:LYS:O	1:A:1079:LYS:NZ	2.38	0.54
1:A:650:ASN:O	1:A:654:ARG:CG	2.56	0.54
1:A:870:ASP:OD1	1:A:873:LYS:HD3	2.08	0.54
2:B:126:VAL:HG22	2:B:189:PRO:HG2	1.89	0.54
1:A:1004:ARG:NH1	1:A:1005:VAL:O	2.38	0.54
1:A:1082:ARG:N	1:A:1082:ARG:CD	2.69	0.53
1:A:235:SER:H	1:A:238:GLN:HE21	1.55	0.53
1:A:917:ALA:HB1	1:A:918:ILE:HG23	1.90	0.53
2:B:15:GLN:HA	2:B:76:PHE:CZ	2.43	0.53
1:A:401:ASP:O	1:A:403:ASP:N	2.41	0.53
2:B:78:ILE:HD11	2:C:273:LEU:CD1	2.39	0.53
1:A:1031:PHE:CE2	1:A:1066:THR:HG21	2.44	0.53
2:C:51:MET:HA	2:C:234:SER:HA	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1013:ARG:HB2	1:A:1014:ILE:HA	1.90	0.53
1:A:219:ILE:HG13	1:A:448:VAL:HG21	1.90	0.53
1:A:946:GLU:O	1:A:950:LEU:HG	2.09	0.53
1:A:614:ARG:HG2	1:A:614:ARG:NH1	2.22	0.53
1:A:708:LEU:HD13	1:A:723:GLN:HG2	1.90	0.53
1:A:968:GLN:HG2	1:A:969:TYR:CE1	2.43	0.53
1:A:435:THR:HA	1:A:505:THR:HA	1.91	0.53
1:A:945:PRO:HB2	1:A:948:VAL:HG22	1.90	0.53
1:A:997:ALA:HB3	1:A:1048:LEU:HD12	1.90	0.53
1:A:8:HIS:NE2	1:A:241:ARG:O	2.38	0.53
1:A:25:ALA:HB3	1:A:26:PRO:HD3	1.91	0.53
2:C:317:ILE:HD11	2:C:363:PRO:HB3	1.90	0.53
1:A:1028:VAL:CA	1:A:1029:MET:HB2	2.38	0.53
1:A:357:PRO:HB2	1:A:407:CYS:HB2	1.90	0.53
1:A:862:LEU:HD11	1:A:902:LEU:HD23	1.91	0.53
1:A:518:ALA:HB2	1:A:551:LEU:HD13	1.91	0.53
1:A:1093:ILE:HG12	1:A:1096:GLN:HG2	1.90	0.52
1:A:434:GLY:O	1:A:506:ARG:N	2.33	0.52
2:B:128:PHE:HB3	2:B:188:LEU:HD11	1.91	0.52
1:A:1020:ASP:HB2	1:A:1021:ASP:HA	1.91	0.52
1:A:894:HIS:HB2	1:A:897:ALA:HB3	1.91	0.52
1:A:997:ALA:CB	1:A:1048:LEU:HD12	2.39	0.52
1:A:265:LYS:HD3	3:D:225:HIS:CE1	2.44	0.52
3:D:9:ILE:HG21	3:D:90:ILE:HG22	1.91	0.52
1:A:11:VAL:HG13	1:A:202:VAL:HB	1.91	0.52
1:A:214:GLU:OE1	1:A:230:ARG:NH2	2.43	0.52
1:A:973:ILE:HG23	1:A:994:ILE:HD13	1.92	0.52
1:A:1027:GLU:HB3	1:A:1029:MET:SD	2.49	0.52
1:A:401:ASP:O	1:A:403:ASP:HB2	2.09	0.52
1:A:432:THR:HG23	1:A:513:GLY:CA	2.39	0.52
1:A:1018:THR:HA	1:A:1025:ARG:CB	2.40	0.52
1:A:1020:ASP:CB	1:A:1021:ASP:HA	2.39	0.52
1:A:967:ASN:O	1:A:968:GLN:HB3	2.10	0.52
4:E:505:LYS:C	4:E:506:THR:OG1	2.47	0.52
1:A:1048:LEU:HD13	1:A:1049:ILE:CA	2.40	0.52
1:A:977:VAL:CG1	1:A:980:VAL:HG13	2.40	0.52
3:D:66:HIS:HB2	3:D:162:HIS:HB3	1.92	0.52
1:A:879:LEU:HD13	1:A:902:LEU:HD22	1.92	0.51
1:A:963:GLY:CA	1:A:967:ASN:CG	2.79	0.51
2:C:281:VAL:CG2	2:C:294:ALA:HB2	2.40	0.51
1:A:18:ILE:HG22	1:A:220:HIS:CE1	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:977:VAL:CG1	1:A:981:ARG:HB2	2.41	0.51
1:A:1013:ARG:HG3	1:A:1014:ILE:CG2	2.35	0.51
1:A:528:LEU:HD13	1:A:537:PRO:HB3	1.93	0.51
1:A:891:LEU:O	1:A:893:PRO:HD3	2.10	0.51
1:A:835:ILE:O	1:A:838:ILE:HG22	2.11	0.51
1:A:650:ASN:O	1:A:654:ARG:HG3	2.11	0.51
2:B:273:LEU:HD21	2:C:108:LEU:HD12	1.92	0.51
1:A:1082:ARG:H	1:A:1082:ARG:CD	2.23	0.50
1:A:518:ALA:HA	1:A:551:LEU:HD22	1.93	0.50
1:A:1018:THR:HG22	1:A:1025:ARG:HB2	1.93	0.50
1:A:1093:ILE:HG13	1:A:1096:GLN:H	1.77	0.50
1:A:964:HIS:N	1:A:967:ASN:OD1	2.43	0.50
1:A:357:PRO:HD2	1:A:410:LYS:HG3	1.92	0.50
2:B:129:THR:HG22	2:B:215:ARG:HB2	1.93	0.50
4:E:622:ASN:O	4:E:623:ASN:HB3	2.11	0.50
1:A:1093:ILE:HD11	1:A:1095:ASP:HB2	1.92	0.50
1:A:921:LEU:HD11	2:C:365:ARG:HG3	1.93	0.50
1:A:58:HIS:ND1	3:D:235:LYS:HB3	2.27	0.50
1:A:1043:GLU:O	1:A:1044:LYS:HB3	2.11	0.50
1:A:1043:GLU:O	1:A:1044:LYS:CB	2.36	0.50
1:A:825:VAL:HG12	1:A:830:GLU:O	2.12	0.50
2:B:275:ASN:HD21	2:B:277:LYS:HE2	1.75	0.50
2:B:53:MET:CE	2:B:230:PHE:HB3	2.42	0.50
1:A:1071:MET:HA	1:A:1075:GLU:CD	2.32	0.50
2:B:126:VAL:HG21	2:B:191:HIS:HB2	1.94	0.50
2:B:103:ARG:HD3	2:C:305:ILE:O	2.12	0.50
1:A:1019:LEU:HD23	1:A:1023:SER:HB2	1.93	0.50
1:A:1048:LEU:HD13	1:A:1049:ILE:N	2.26	0.50
1:A:969:TYR:CD1	1:A:969:TYR:N	2.79	0.49
1:A:1014:ILE:O	1:A:1014:ILE:HG12	2.11	0.49
1:A:1098:LEU:O	1:A:1099:ASN:HB2	2.12	0.49
2:C:279:ARG:O	2:C:321:VAL:HG12	2.12	0.49
4:E:530:LEU:HD21	4:E:579:LEU:HB2	1.94	0.49
1:A:66:VAL:HG11	1:A:88:ALA:HB3	1.93	0.49
2:C:47:THR:HG22	2:C:116:PHE:CZ	2.46	0.49
1:A:1071:MET:HB2	1:A:1075:GLU:CG	2.42	0.49
2:B:103:ARG:O	2:C:305:ILE:HD12	2.13	0.49
1:A:1047:ILE:O	1:A:1048:LEU:HB2	2.12	0.49
2:B:52:GLU:N	2:B:233:THR:O	2.46	0.49
1:A:1043:GLU:HG3	1:A:1044:LYS:HG3	1.94	0.49
2:C:32:ASN:CB	2:C:69:THR:HG23	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:946:GLU:HA	1:A:949:VAL:HG12	1.94	0.49
1:A:977:VAL:O	1:A:980:VAL:HG12	2.12	0.49
4:E:554:LEU:CD1	4:E:586:LEU:HD11	2.42	0.49
1:A:1088:LEU:HD22	1:A:1089:THR:O	2.12	0.49
4:E:518:ILE:HG23	4:E:525:ALA:HA	1.94	0.49
1:A:1106:GLU:HB3	1:A:1107:PRO:HD3	1.95	0.49
1:A:109:TYR:HB3	1:A:114:PRO:HA	1.93	0.49
1:A:359:GLY:H	1:A:406:PHE:HA	1.78	0.49
1:A:823:PHE:CD2	1:A:833:TYR:HA	2.48	0.49
1:A:13:SER:HA	1:A:27:LEU:HD11	1.94	0.48
1:A:1133:THR:HB	1:A:1134:TRP:CE3	2.48	0.48
1:A:170:LEU:HD11	1:A:196:VAL:HG21	1.96	0.48
1:A:991:GLY:N	1:A:1054:VAL:O	2.46	0.48
1:A:1117:LEU:HD13	1:A:1118:TYR:C	2.34	0.48
1:A:289:GLU:O	1:A:293:VAL:HG23	2.13	0.48
1:A:833:TYR:CZ	1:A:957:LEU:HD13	2.47	0.48
2:B:184:ILE:HD13	2:B:188:LEU:HD21	1.95	0.48
1:A:1077:ARG:HG2	1:A:1082:ARG:HE	1.78	0.48
1:A:999:LEU:HD13	1:A:1000:VAL:N	2.29	0.48
3:D:52:LEU:HD21	3:D:82:VAL:HG21	1.95	0.48
1:A:559:LEU:HD13	1:A:560:ARG:N	2.29	0.48
1:A:816:ILE:HG23	1:A:849:ILE:CG2	2.42	0.48
1:A:18:ILE:HG22	1:A:220:HIS:NE2	2.28	0.48
1:A:289:GLU:HG3	1:A:338:PRO:HG3	1.96	0.48
1:A:797:VAL:O	1:A:801:VAL:HG13	2.13	0.48
1:A:798:VAL:HG11	1:A:1023:SER:O	2.14	0.48
1:A:277:PHE:N	1:A:277:PHE:CD1	2.82	0.48
1:A:433:PHE:CD1	1:A:505:THR:HG21	2.49	0.48
2:C:17:VAL:HG22	2:C:53:MET:CG	2.44	0.48
1:A:668:TRP:HA	1:A:740:LEU:CD1	2.44	0.47
1:A:810:LYS:HA	1:A:811:ILE:HB	1.95	0.47
1:A:977:VAL:HB	1:A:981:ARG:HB2	1.95	0.47
2:B:10:LEU:O	2:B:14:LEU:HB2	2.15	0.47
2:B:321:VAL:HG22	2:B:325:LEU:HD22	1.96	0.47
2:C:126:VAL:HG13	2:C:218:ILE:HB	1.95	0.47
1:A:1049:ILE:HB	1:A:1076:ALA:HB2	1.95	0.47
2:B:281:VAL:HG22	2:B:294:ALA:CB	2.42	0.47
3:D:229:LEU:HD22	3:D:239:CYS:SG	2.53	0.47
4:E:541:LEU:HD23	4:E:599:PRO:HG2	1.97	0.47
2:B:22:GLY:O	2:B:24:ARG:N	2.43	0.47
1:A:864:ASP:O	1:A:868:ARG:HD3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:MET:HA	1:A:216:ARG:NH2	2.30	0.47
1:A:517:ILE:HD12	1:A:554:PHE:CE2	2.50	0.47
2:B:214:LEU:HD11	2:B:225:ALA:HB1	1.96	0.47
4:E:541:LEU:HA	4:E:599:PRO:HG2	1.97	0.47
1:A:324:ARG:HD2	1:A:328:GLU:OE2	2.15	0.47
1:A:576:ARG:O	1:A:580:GLY:N	2.47	0.47
2:B:138:LEU:HD13	2:B:182:MET:HG3	1.97	0.47
1:A:1077:ARG:C	1:A:1079:LYS:H	2.19	0.47
1:A:572:ILE:O	1:A:575:ARG:HB2	2.15	0.46
1:A:66:VAL:HG21	1:A:269:VAL:CG2	2.45	0.46
2:C:159:LEU:HD13	2:C:241:PHE:CB	2.44	0.46
1:A:63:LYS:HB2	3:D:232:VAL:HG21	1.96	0.46
1:A:924:PHE:HB2	1:A:925:GLY:HA2	1.93	0.46
2:B:96:ARG:NH2	2:C:299:GLN:O	2.48	0.46
1:A:1119:TYR:CE1	4:E:618:ILE:HD12	2.50	0.46
1:A:1121:ARG:HD2	4:E:618:ILE:HD11	1.97	0.46
1:A:200:ASN:ND2	1:A:241:ARG:HD2	2.31	0.46
1:A:459:ILE:CD1	1:A:491:VAL:HG22	2.45	0.46
1:A:964:HIS:O	1:A:967:ASN:OD1	2.33	0.46
2:C:156:ASN:O	2:C:197:ARG:N	2.46	0.46
1:A:1021:ASP:O	1:A:1023:SER:N	2.49	0.46
1:A:1048:LEU:HD21	1:A:1050:VAL:CG1	2.45	0.46
1:A:830:GLU:O	1:A:831:ILE:HD13	2.15	0.46
1:A:892:GLY:HA3	1:A:898:LEU:CG	2.46	0.46
3:D:79:PHE:CD2	3:D:114:LEU:HD11	2.51	0.46
3:D:54:PRO:HD3	3:D:73:LEU:O	2.15	0.46
2:C:197:ARG:O	2:C:201:ILE:HG12	2.16	0.46
2:C:99:VAL:HB	2:C:106:PHE:HB2	1.96	0.46
1:A:1049:ILE:HD12	1:A:1076:ALA:HB1	1.98	0.46
1:A:1079:LYS:CE	1:A:1155:VAL:HG22	2.46	0.46
1:A:650:ASN:O	1:A:654:ARG:HG2	2.16	0.46
2:B:11:LEU:HD12	2:B:11:LEU:HA	1.85	0.46
2:C:167:LEU:HD12	2:C:184:ILE:HG12	1.97	0.46
1:A:1073:ILE:O	1:A:1073:ILE:HD13	2.16	0.46
2:B:21:LEU:HD22	2:B:72:ALA:HB3	1.97	0.46
2:B:78:ILE:HD11	2:C:273:LEU:HD11	1.97	0.46
1:A:969:TYR:CE2	1:A:1141:ARG:CZ	2.99	0.45
2:B:292:ILE:HD12	2:B:304:GLU:HB2	1.98	0.45
1:A:321:TYR:CD2	1:A:369:LEU:HD11	2.51	0.45
1:A:371:ALA:HB1	1:A:377:THR:HG23	1.97	0.45
1:A:959:LEU:C	1:A:959:LEU:HD22	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1042:LEU:HD23	1:A:1070:VAL:HG21	1.97	0.45
1:A:1084:LEU:HD23	1:A:1115:VAL:HG13	1.98	0.45
1:A:66:VAL:HG21	1:A:269:VAL:HG21	1.98	0.45
1:A:3:GLU:N	1:A:4:PRO:CD	2.79	0.45
2:C:52:GLU:N	2:C:233:THR:O	2.46	0.45
1:A:1093:ILE:HG13	1:A:1094:ASP:N	2.31	0.45
1:A:528:LEU:HD13	1:A:537:PRO:CB	2.47	0.45
2:B:184:ILE:HG21	2:B:188:LEU:HD22	1.99	0.45
2:B:258:ALA:HB2	2:B:308:VAL:HG22	1.99	0.45
1:A:393:ASN:ND2	1:A:706:ASP:OD2	2.48	0.45
1:A:586:ILE:HD13	1:A:774:LEU:HD13	1.99	0.45
1:A:838:ILE:CG2	1:A:841:VAL:HB	2.46	0.45
3:D:17:GLY:N	3:D:62:ALA:HB2	2.32	0.45
1:A:391:PHE:CZ	1:A:402:PHE:CD1	3.04	0.45
1:A:436:MET:HE3	1:A:504:VAL:O	2.17	0.45
3:D:61:GLU:O	3:D:65:VAL:HG23	2.16	0.45
1:A:1100:ARG:HA	1:A:1103:GLN:HG2	1.99	0.45
1:A:869:THR:O	1:A:869:THR:HG23	2.16	0.45
2:C:135:MET:HG3	2:C:207:LEU:HD21	1.98	0.45
1:A:919:GLY:O	2:C:364:MET:HG3	2.16	0.45
1:A:1098:LEU:O	1:A:1099:ASN:CB	2.64	0.45
1:A:45:THR:O	1:A:45:THR:HG22	2.17	0.45
2:C:195:VAL:HG12	2:C:236:LEU:HD11	1.98	0.45
3:D:11:LEU:CD1	3:D:35:ALA:HB2	2.36	0.45
1:A:1077:ARG:HH11	1:A:1113:ILE:HD11	1.81	0.45
2:B:67:ALA:HB1	2:B:113:ALA:CB	2.47	0.45
1:A:1093:ILE:HG13	1:A:1095:ASP:N	2.32	0.44
1:A:793:ASN:O	1:A:797:VAL:HG23	2.17	0.44
1:A:810:LYS:HA	1:A:811:ILE:C	2.37	0.44
1:A:72:VAL:CG2	1:A:84:LEU:HD12	2.46	0.44
2:B:224:ARG:HA	2:B:232:PHE:O	2.17	0.44
2:C:17:VAL:HG22	2:C:53:MET:HG3	2.00	0.44
4:E:556:LEU:HD22	4:E:564:ASN:HB2	1.99	0.44
1:A:318:ARG:N	1:A:319:PRO:HD2	2.32	0.44
1:A:1124:ALA:HB2	4:E:611:LEU:HG	1.99	0.44
1:A:345:MET:HB3	1:A:376:ILE:HD11	2.00	0.44
1:A:968:GLN:HG2	1:A:969:TYR:CD2	2.53	0.44
3:D:91:ARG:HG3	3:D:124:PHE:CD1	2.52	0.44
1:A:1086:ILE:HD12	1:A:1117:LEU:HD22	2.00	0.44
3:D:17:GLY:HA3	3:D:59:ASP:CB	2.47	0.44
2:B:176:ARG:CB	2:B:361:VAL:HG12	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1037:LYS:HA	1:A:1037:LYS:HE2	1.98	0.44
1:A:42:THR:HG22	1:A:67:GLY:HA3	1.99	0.44
1:A:822:HIS:CD2	1:A:823:PHE:CD1	3.06	0.44
1:A:924:PHE:CG	1:A:925:GLY:HA3	2.52	0.44
1:A:801:VAL:O	1:A:805:TRP:HD1	2.00	0.44
2:C:126:VAL:HG11	2:C:191:HIS:CB	2.46	0.44
1:A:72:VAL:HA	1:A:116:ILE:HG13	2.00	0.44
2:B:285:VAL:HG12	2:B:315:MET:O	2.18	0.44
1:A:1101:LEU:HD13	1:A:1101:LEU:C	2.38	0.43
1:A:1100:ARG:O	1:A:1103:GLN:HG2	2.18	0.43
1:A:261:VAL:HG13	3:D:241:TRP:CH2	2.53	0.43
1:A:824:HIS:O	1:A:832:VAL:HG22	2.18	0.43
1:A:892:GLY:HA3	1:A:898:LEU:HD11	1.99	0.43
1:A:1020:ASP:CA	1:A:1021:ASP:O	2.58	0.43
1:A:1117:LEU:HD13	1:A:1118:TYR:N	2.32	0.43
1:A:779:PRO:HA	1:A:782:PHE:HB3	2.00	0.43
1:A:841:VAL:HG12	1:A:842:GLY:O	2.18	0.43
1:A:847:GLU:O	1:A:850:ILE:HG12	2.19	0.43
1:A:999:LEU:C	1:A:999:LEU:HD13	2.39	0.43
1:A:973:ILE:CG1	1:A:1079:LYS:HD2	2.48	0.43
2:B:154:TYR:HA	2:B:237:VAL:HG21	1.99	0.43
2:C:67:ALA:HB1	2:C:113:ALA:CB	2.49	0.43
1:A:1026:LEU:HD13	1:A:1063:LEU:H	1.82	0.43
1:A:1106:GLU:HA	1:A:1134:TRP:NE1	2.33	0.43
1:A:964:HIS:N	1:A:967:ASN:CG	2.72	0.43
2:C:136:LYS:HA	2:C:207:LEU:HD23	2.00	0.43
2:C:256:LEU:HD11	2:C:285:VAL:HG21	2.00	0.43
1:A:586:ILE:HD13	1:A:774:LEU:CD1	2.48	0.43
1:A:9:LEU:HB2	1:A:199:THR:HG22	2.00	0.43
1:A:1057:ASP:HB2	1:A:1063:LEU:HA	1.99	0.43
1:A:400:PRO:C	1:A:402:PHE:N	2.72	0.43
1:A:429:GLN:CB	1:A:538:VAL:HG12	2.49	0.43
2:C:208:ASP:O	2:C:210:GLY:N	2.45	0.43
2:C:317:ILE:HD11	2:C:363:PRO:CB	2.48	0.43
1:A:801:VAL:O	1:A:805:TRP:CD1	2.71	0.43
3:D:17:GLY:HA3	3:D:59:ASP:HB2	2.01	0.43
1:A:892:GLY:HA3	1:A:898:LEU:CD1	2.49	0.43
1:A:968:GLN:HG2	1:A:969:TYR:CD1	2.53	0.43
1:A:975:ARG:O	1:A:976:TYR:CD1	2.69	0.43
2:C:282:ARG:NE	2:C:366:LEU:HD23	2.34	0.43
1:A:963:GLY:CA	1:A:967:ASN:OD1	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:542:ASN:OD1	4:E:600:LEU:HD13	2.19	0.43
1:A:1093:ILE:CD1	1:A:1096:GLN:HG2	2.49	0.42
1:A:130:LEU:HB2	1:A:166:TYR:HD1	1.84	0.42
1:A:780:ALA:HB3	1:A:781:GLU:OE2	2.18	0.42
1:A:796:LYS:O	1:A:800:LEU:HG	2.19	0.42
2:B:158:MET:SD	2:B:169:THR:HB	2.59	0.42
1:A:973:ILE:HG22	1:A:994:ILE:HG21	2.00	0.42
1:A:19:ASP:HA	1:A:216:ARG:HD2	2.02	0.42
1:A:276:TYR:CE2	1:A:399:MET:HG3	2.54	0.42
1:A:1088:LEU:HD23	1:A:1089:THR:N	2.35	0.42
1:A:595:LYS:HD3	1:A:777:HIS:NE2	2.34	0.42
2:C:258:ALA:HB3	2:C:263:LEU:HD22	2.01	0.42
1:A:19:ASP:HB2	1:A:213:HIS:NE2	2.35	0.42
1:A:820:LEU:HD12	1:A:824:HIS:CD2	2.55	0.42
1:A:835:ILE:HG12	1:A:846:ILE:HG22	2.02	0.42
1:A:547:GLU:OE2	1:A:553:LYS:HG2	2.20	0.42
1:A:825:VAL:HG23	1:A:825:VAL:O	2.20	0.42
1:A:838:ILE:HG23	1:A:841:VAL:HB	2.02	0.42
1:A:865:LEU:O	1:A:869:THR:HG22	2.19	0.42
4:E:504:GLU:HB2	4:E:505:LYS:HB3	2.02	0.42
1:A:833:TYR:OH	1:A:959:LEU:HD11	2.20	0.42
1:A:968:GLN:CG	1:A:969:TYR:CZ	3.01	0.42
1:A:1130:PHE:CE2	1:A:1132:ALA:CB	3.03	0.41
1:A:237:GLN:HE21	1:A:241:ARG:HH22	1.68	0.41
1:A:842:GLY:O	1:A:846:ILE:HG23	2.19	0.41
1:A:1077:ARG:CG	1:A:1082:ARG:HE	2.32	0.41
1:A:925:GLY:O	1:A:926:VAL:HG12	2.20	0.41
1:A:946:GLU:CA	1:A:949:VAL:HG12	2.51	0.41
2:B:51:MET:HA	2:B:234:SER:HA	2.02	0.41
1:A:869:THR:CG2	1:A:874:LEU:HD12	2.39	0.41
1:A:924:PHE:HD2	1:A:925:GLY:HA3	1.82	0.41
1:A:1027:GLU:O	1:A:1029:MET:HG2	2.20	0.41
1:A:950:LEU:HD22	1:A:961:LEU:O	2.20	0.41
1:A:1018:THR:HA	1:A:1025:ARG:HB2	2.01	0.41
1:A:844:GLY:O	1:A:847:GLU:HG2	2.19	0.41
2:C:147:ALA:N	2:C:173:ASP:HB3	2.35	0.41
2:C:90:VAL:HG13	2:C:98:LEU:O	2.20	0.41
1:A:1037:LYS:O	1:A:1041:LEU:HG	2.20	0.41
1:A:1053:GLN:O	1:A:1066:THR:HG22	2.21	0.41
1:A:72:VAL:HG22	1:A:84:LEU:HD12	2.02	0.41
1:A:866:CYS:HB3	1:A:906:LEU:HD23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:282:ARG:CD	2:C:366:LEU:HD23	2.50	0.41
1:A:1078:GLU:O	1:A:1080:TYR:C	2.59	0.41
1:A:330:GLN:O	1:A:334:GLN:HG3	2.21	0.41
1:A:1028:VAL:HA	1:A:1029:MET:HG2	1.97	0.41
1:A:204:PHE:CE1	1:A:239:TYR:HB3	2.56	0.41
1:A:862:LEU:CD2	1:A:901:SER:OG	2.68	0.41
2:B:108:LEU:HD11	2:C:273:LEU:HD21	2.03	0.41
2:B:321:VAL:HA	2:B:324:VAL:CG1	2.50	0.41
2:C:279:ARG:HB3	2:C:321:VAL:HG12	2.03	0.41
1:A:69:ASP:HA	1:A:84:LEU:O	2.21	0.41
3:D:17:GLY:H	3:D:62:ALA:HB2	1.86	0.41
1:A:196:VAL:HG22	1:A:255:GLU:OE2	2.21	0.41
2:B:111:LEU:HA	2:B:111:LEU:HD12	1.97	0.41
3:D:109:TYR:O	3:D:113:LEU:HG	2.21	0.41
1:A:966:ILE:O	1:A:966:ILE:HG23	2.21	0.41
2:B:222:ASN:HA	2:B:235:LYS:HA	2.02	0.41
1:A:1048:LEU:HD13	1:A:1048:LEU:C	2.41	0.40
1:A:1079:LYS:NZ	1:A:1155:VAL:HA	2.35	0.40
1:A:100:LEU:HD21	1:A:120:TRP:HB3	2.03	0.40
1:A:147:ASN:O	1:A:151:VAL:HG23	2.21	0.40
1:A:14:ASP:HB2	1:A:504:VAL:HG13	2.04	0.40
1:A:775:LYS:O	1:A:779:PRO:HD3	2.18	0.40
1:A:966:ILE:HG21	1:A:998:GLY:CA	2.50	0.40
1:A:1093:ILE:HD12	1:A:1095:ASP:HB2	2.03	0.40
1:A:790:ASP:O	1:A:797:VAL:HG23	2.21	0.40
1:A:814:PRO:HG2	1:A:885:SER:OG	2.21	0.40
1:A:920:GLN:HG3	1:A:921:LEU:O	2.22	0.40
1:A:972:GLU:HG2	1:A:1155:VAL:HG23	2.03	0.40
1:A:977:VAL:HG12	1:A:980:VAL:CG1	2.50	0.40
3:D:16:THR:HG22	3:D:58:VAL:CA	2.44	0.40
1:A:1088:LEU:HD21	1:A:1092:GLN:HB3	2.02	0.40
1:A:69:ASP:OD1	1:A:85:THR:HG23	2.21	0.40
2:B:69:THR:HB	2:B:111:LEU:O	2.21	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 PDB entries followed by that with respect to all EM entries.

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	1145/1160 (99%)	1052 (92%)	62 (5%)	31 (3%)	6	40
2	B	364/366 (100%)	346 (95%)	13 (4%)	5 (1%)	13	54
2	C	364/366 (100%)	343 (94%)	18 (5%)	3 (1%)	22	67
3	D	214/243 (88%)	191 (89%)	18 (8%)	5 (2%)	7	43
4	E	118/144 (82%)	112 (95%)	4 (3%)	2 (2%)	11	50
All	All	2205/2279 (97%)	2044 (93%)	115 (5%)	46 (2%)	12	45

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	279	PRO
1	A	810	LYS
1	A	968	GLN
1	A	970	LEU
1	A	997	ALA
1	A	1007	VAL
1	A	1023	SER
1	A	1035	LEU
1	A	1080	TYR
1	A	1093	ILE
2	B	23	GLY
2	C	209	GLY
2	C	239	GLY
3	D	68	ILE
3	D	182	GLN
1	A	401	ASP
1	A	969	TYR
1	A	1009	LYS
1	A	1021	ASP
1	A	1029	MET
1	A	1034	ALA

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Mol	Chain	Res	Type
1	A	1099	ASN
1	A	1148	GLY
1	A	2	SER
1	A	1013	ARG
1	A	1081	ALA
1	A	1131	GLY
1	A	1133	THR
2	B	287	GLU
2	C	153	TYR
3	D	186	PRO
3	D	187	LEU
3	D	210	SER
4	E	533	PRO
1	A	811	ILE
1	A	925	GLY
1	A	940	SER
2	B	240	ARG
4	E	506	THR
1	A	1008	THR
1	A	1022	ARG
1	A	1048	LEU
1	A	543	LYS
1	A	1111	GLY
2	B	22	GLY
2	B	102	GLY

### 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 PDB entries followed by that with respect to all EM entries.

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	955/965 (99%)	862 (90%)	93 (10%)	9	35
2	B	313/313 (100%)	270 (86%)	43 (14%)	4	23
2	C	313/313 (100%)	263 (84%)	50 (16%)	3	18
3	D	179/200 (90%)	169 (94%)	10 (6%)	25	57
4	E	100/122 (82%)	87 (87%)	13 (13%)	5	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1860/1913 (97%)	1651 (89%)	209 (11%)	11	29

All (209) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	3	GLU
1	A	7	VAL
1	A	21	LEU
1	A	29	LYS
1	A	39	LEU
1	A	69	ASP
1	A	75	ASP
1	A	84	LEU
1	A	90	ASN
1	A	99	LEU
1	A	100	LEU
1	A	124	LEU
1	A	138	ASP
1	A	144	LEU
1	A	145	ARG
1	A	147	ASN
1	A	188	LEU
1	A	216	ARG
1	A	224	THR
1	A	225	LEU
1	A	240	MET
1	A	249	LEU
1	A	262	GLU
1	A	265	LYS
1	A	285	ASP
1	A	287	SER
1	A	298	GLU
1	A	329	LEU
1	A	342	LEU
1	A	351	SER
1	A	369	LEU
1	A	399	MET
1	A	405	ASP
1	A	414	VAL
1	A	418	VAL
1	A	421	MET

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Mol	Chain	Res	Type
1	A	424	ARG
1	A	432	THR
1	A	436	MET
1	A	443	ARG
1	A	456	VAL
1	A	481	LEU
1	A	546	VAL
1	A	557	LEU
1	A	559	LEU
1	A	571	MET
1	A	576	ARG
1	A	578	LYS
1	A	594	LYS
1	A	603	SER
1	A	613	SER
1	A	614	ARG
1	A	643	LEU
1	A	658	ARG
1	A	666	VAL
1	A	671	GLU
1	A	697	LEU
1	A	707	MET
1	A	723	GLN
1	A	757	ASN
1	A	774	LEU
1	A	810	LYS
1	A	868	ARG
1	A	918	ILE
1	A	922	ASP
1	A	959	LEU
1	A	964	HIS
1	A	968	GLN
1	A	969	TYR
1	A	974	GLU
1	A	976	TYR
1	A	1004	ARG
1	A	1005	VAL
1	A	1007	VAL
1	A	1009	LYS
1	A	1010	ARG
1	A	1013	ARG
1	A	1014	ILE

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Mol	Chain	Res	Type
1	A	1017	CYS
1	A	1020	ASP
1	A	1021	ASP
1	A	1025	ARG
1	A	1029	MET
1	A	1030	LEU
1	A	1031	PHE
1	A	1035	LEU
1	A	1037	LYS
1	A	1044	LYS
1	A	1073	ILE
1	A	1079	LYS
1	A	1082	ARG
1	A	1125	ARG
2	B	1	MET
2	B	5	VAL
2	B	14	LEU
2	B	39	ASP
2	B	42	LEU
2	B	59	LEU
2	B	70	VAL
2	B	88	ILE
2	B	103	ARG
2	B	104	SER
2	B	110	THR
2	B	111	LEU
2	B	123	GLN
2	B	125	GLU
2	B	137	ARG
2	B	138	LEU
2	B	143	GLN
2	B	167	LEU
2	B	170	VAL
2	B	176	ARG
2	B	188	LEU
2	B	191	HIS
2	B	195	VAL
2	B	207	LEU
2	B	233	THR
2	B	236	LEU
2	B	237	VAL
2	B	238	ASP

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Mol	Chain	Res	Type
2	B	240	ARG
2	B	257	GLU
2	B	275	ASN
2	B	282	ARG
2	B	289	GLN
2	B	306	LEU
2	B	308	VAL
2	B	319	PHE
2	B	325	LEU
2	B	327	VAL
2	B	328	LEU
2	B	331	LEU
2	B	332	LYS
2	B	364	MET
2	B	366	LEU
2	C	5	VAL
2	C	21	LEU
2	C	29	ILE
2	C	42	LEU
2	C	49	LEU
2	C	57	VAL
2	C	59	LEU
2	C	69	THR
2	C	88	ILE
2	C	103	ARG
2	C	105	ARG
2	C	108	LEU
2	C	110	THR
2	C	118	ASN
2	C	123	GLN
2	C	126	VAL
2	C	137	ARG
2	C	138	LEU
2	C	142	THR
2	C	151	VAL
2	C	162	THR
2	C	163	GLU
2	C	167	LEU
2	C	170	VAL
2	C	176	ARG
2	C	188	LEU
2	C	193	VAL

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Mol	Chain	Res	Type
2	C	197	ARG
2	C	200	VAL
2	C	203	LEU
2	C	205	ARG
2	C	207	LEU
2	C	211	ASP
2	C	216	VAL
2	C	233	THR
2	C	236	LEU
2	C	237	VAL
2	C	246	ARG
2	C	248	LEU
2	C	262	LEU
2	C	273	LEU
2	C	281	VAL
2	C	306	LEU
2	C	324	VAL
2	C	325	LEU
2	C	328	LEU
2	C	340	LEU
2	C	355	GLN
2	C	360	VAL
2	C	366	LEU
3	D	13	THR
3	D	16	THR
3	D	42	ARG
3	D	59	ASP
3	D	70	ASP
3	D	78	THR
3	D	144	SER
3	D	157	SER
3	D	212	LEU
3	D	234	LYS
4	E	505	LYS
4	E	509	LEU
4	E	520	ARG
4	E	559	SER
4	E	571	LYS
4	E	572	LEU
4	E	576	LEU
4	E	597	ARG
4	E	609	GLU

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Mol	Chain	Res	Type
4	E	610	LYS
4	E	613	GLN
4	E	621	ASP
4	E	623	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	ASN
1	A	95	GLN
1	A	147	ASN
1	A	237	GLN
1	A	238	GLN
1	A	280	GLN
1	A	413	GLN
1	A	417	HIS
1	A	650	ASN
1	A	723	GLN
1	A	757	ASN
1	A	824	HIS
1	A	942	GLN
1	A	964	HIS
1	A	968	GLN
1	A	1039	GLN
2	B	16	GLN
2	B	186	GLN
2	B	221	ASN
2	B	275	ASN
2	B	288	ASN
2	C	156	ASN
2	C	355	GLN
3	D	225	HIS

### 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 [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.