



# Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 05:47 am BST

PDB ID : 3BGW  
Title : The Structure Of A DnaB-Like Replicative Helicase And Its Interactions With Primase  
Authors : Wang, G.; Klein, M.G.; Tokonzaba, E.; Zhang, Y.; Holden, L.G.; Chen, X.S.  
Deposited on : 2007-11-27  
Resolution : 3.91 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

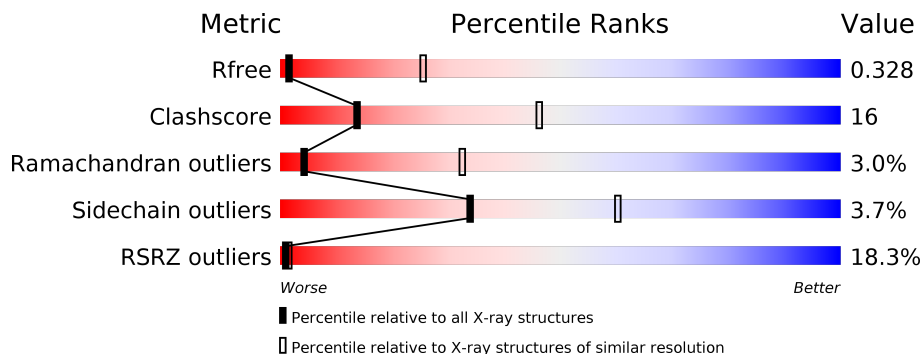
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.91 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	1019 (4.18-3.66)
Clashscore	141614	1016 (4.16-3.68)
Ramachandran outliers	138981	1039 (4.18-3.66)
Sidechain outliers	138945	1032 (4.18-3.66)
RSRZ outliers	127900	1002 (4.20-3.64)

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	444	
1	B	444	
1	C	444	
1	D	444	
1	E	444	
1	F	444	

## 2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 19724 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 DNAB-Like Replicative Helicase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	419	3298	2062	571	653	12	0	0	0
1	B	419	3298	2062	571	653	12	0	0	0
1	C	419	3298	2062	571	653	12	0	0	0
1	D	409	3234	2029	561	632	12	0	0	0
1	E	419	3298	2062	571	653	12	0	0	0
1	F	419	3298	2062	571	653	12	0	0	0

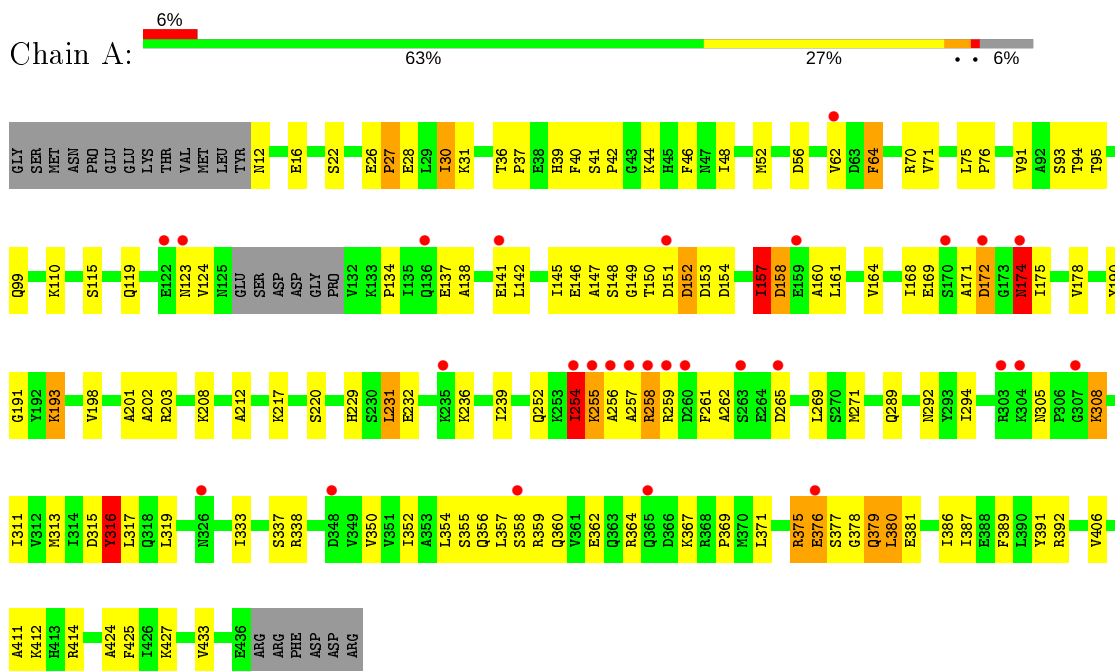
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP Q38152
A	0	SER	-	EXPRESSION TAG	UNP Q38152
B	-1	GLY	-	EXPRESSION TAG	UNP Q38152
B	0	SER	-	EXPRESSION TAG	UNP Q38152
C	-1	GLY	-	EXPRESSION TAG	UNP Q38152
C	0	SER	-	EXPRESSION TAG	UNP Q38152
D	-1	GLY	-	EXPRESSION TAG	UNP Q38152
D	0	SER	-	EXPRESSION TAG	UNP Q38152
E	-1	GLY	-	EXPRESSION TAG	UNP Q38152
E	0	SER	-	EXPRESSION TAG	UNP Q38152
F	-1	GLY	-	EXPRESSION TAG	UNP Q38152
F	0	SER	-	EXPRESSION TAG	UNP Q38152

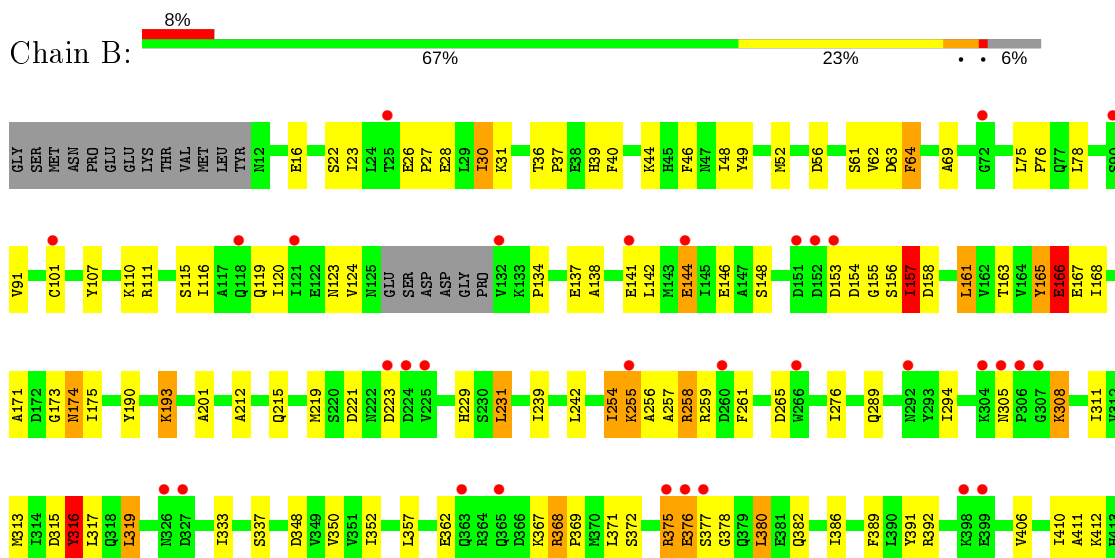
### 3 Residue-property plots

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

#### • Molecule 1: DNAB-Like Replicative Helicase



#### • Molecule 1: DNAB-Like Replicative Helicase







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	114.63Å 184.41Å 184.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.81 – 3.91 38.80 – 3.91	Depositor EDS
% Data completeness (in resolution range)	97.5 (38.81-3.91) 97.4 (38.80-3.91)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	12.68 (at 3.87Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.338 , 0.349 0.321 , 0.328	Depositor DCC
$R_{free}$ test set	1750 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	65.0	Xtrriage
Anisotropy	0.385	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 140.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.54$ , $\langle L^2 \rangle = 0.38$	Xtrriage
Estimated twinning fraction	0.000 for -h,l,k	Xtrriage
$F_o, F_c$ correlation	0.81	EDS
Total number of atoms	19724	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	119.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.32	1/3345 (0.0%)	0.41	0/4507
1	B	0.26	0/3345	0.40	0/4507
1	C	0.30	2/3345 (0.1%)	0.39	0/4507
1	D	0.27	0/3280	0.39	0/4417
1	E	0.32	2/3345 (0.1%)	0.41	0/4507
1	F	0.34	4/3345 (0.1%)	0.42	1/4507 (0.0%)
All	All	0.30	9/20005 (0.0%)	0.40	1/26952 (0.0%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	173	GLY	C-O	-8.20	1.10	1.23
1	F	174	ASN	CB-CG	-7.97	1.32	1.51
1	E	159	GLU	CD-OE2	6.62	1.32	1.25
1	A	174	ASN	CB-CG	-6.20	1.36	1.51
1	C	174	ASN	CB-CG	-6.08	1.37	1.51
1	C	174	ASN	CG-OD1	-5.54	1.11	1.24
1	F	174	ASN	C-O	-5.23	1.13	1.23
1	F	174	ASN	CA-C	-5.16	1.39	1.52
1	F	174	ASN	CA-CB	-5.13	1.39	1.53

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	174	ASN	N-CA-C	6.07	127.39	111.00

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	3298	0	3279	138	0
1	B	3298	0	3279	119	0
1	C	3298	0	3279	121	0
1	D	3234	0	3234	107	0
1	E	3298	0	3279	114	0
1	F	3298	0	3277	127	0
All	All	19724	0	19627	626	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 16.

All (626) 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:D:52:MET:HG3	1:D:62:VAL:HG11	1.28	1.08
1:E:232:GLU:OE2	1:F:414:ARG:NH1	1.87	1.07
1:D:259:ARG:HB2	1:E:170:SER:O	1.52	1.07
1:E:168:ILE:HG13	1:E:169:GLU:H	1.10	1.06
1:F:52:MET:HG3	1:F:62:VAL:HG11	1.37	1.05
1:A:174:ASN:N	1:A:174:ASN:OD1	1.63	1.05
1:A:315:ASP:O	1:A:316:TYR:HB2	1.54	1.05
1:C:299:ARG:NH2	1:D:31:LYS:HB3	1.73	1.03
1:F:315:ASP:O	1:F:316:TYR:HB2	1.58	1.02
1:C:315:ASP:O	1:C:316:TYR:HB2	1.57	1.02
1:D:315:ASP:O	1:D:316:TYR:HB2	1.59	1.02
1:A:190:TYR:OH	1:F:256:ALA:HB2	1.58	1.02
1:B:315:ASP:O	1:B:316:TYR:HB2	1.57	1.01
1:E:52:MET:HG3	1:E:62:VAL:HG11	1.43	1.00
1:C:52:MET:HG3	1:C:62:VAL:HG11	1.44	0.99
1:C:258:ARG:HG2	1:D:168:ILE:CG2	1.91	0.99
1:E:315:ASP:O	1:E:316:TYR:HB2	1.58	0.99
1:A:232:GLU:OE2	1:B:414:ARG:NH1	1.97	0.97
1:E:239:ILE:CD1	1:F:161:LEU:HG	1.94	0.96
1:E:157:ILE:HG13	1:E:158:ASP:H	1.31	0.95
1:C:299:ARG:HH22	1:D:31:LYS:HB3	1.27	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:239:ILE:HD13	1:F:161:LEU:HG	1.46	0.94
1:A:157:ILE:HG23	1:A:158:ASP:H	1.29	0.94
1:E:377:SER:HB2	1:E:380:LEU:HB2	1.48	0.94
1:B:52:MET:HG3	1:B:62:VAL:HG11	1.46	0.94
1:D:377:SER:HB2	1:D:380:LEU:HB2	1.50	0.93
1:A:257:ALA:HA	1:B:173:GLY:HA2	1.51	0.93
1:C:377:SER:HB2	1:C:380:LEU:HB2	1.50	0.93
1:A:377:SER:HB2	1:A:380:LEU:HB2	1.50	0.92
1:B:377:SER:HB2	1:B:380:LEU:HB2	1.51	0.91
1:F:377:SER:HB2	1:F:380:LEU:HB2	1.53	0.90
1:C:258:ARG:HH22	1:C:265:ASP:HB2	1.39	0.88
1:E:168:ILE:HG13	1:E:169:GLU:N	1.89	0.87
1:F:317:LEU:HD21	1:F:380:LEU:HD21	1.56	0.87
1:A:258:ARG:HG2	1:B:168:ILE:HG23	1.54	0.87
1:E:18:ALA:HB2	1:F:65:THR:HG21	1.59	0.84
1:A:258:ARG:HH22	1:A:265:ASP:HB2	1.43	0.84
1:A:157:ILE:HG23	1:A:158:ASP:N	1.93	0.83
1:E:317:LEU:HD21	1:E:380:LEU:HD21	1.59	0.83
1:A:52:MET:HG3	1:A:62:VAL:HG11	1.60	0.82
1:D:273:ILE:HG23	1:E:161:LEU:HD11	1.61	0.82
1:E:157:ILE:HG13	1:E:158:ASP:N	1.95	0.82
1:D:317:LEU:HD21	1:D:380:LEU:HD21	1.62	0.82
1:F:258:ARG:HH22	1:F:265:ASP:HB2	1.44	0.82
1:C:317:LEU:HD21	1:C:380:LEU:HD21	1.60	0.81
1:D:52:MET:HG3	1:D:62:VAL:CG1	2.10	0.81
1:E:52:MET:HG3	1:E:62:VAL:CG1	2.10	0.81
1:B:258:ARG:HH22	1:B:265:ASP:HB2	1.46	0.81
1:B:317:LEU:HD21	1:B:380:LEU:HD21	1.63	0.80
1:D:258:ARG:HH22	1:D:265:ASP:HB2	1.43	0.80
1:A:75:LEU:N	1:A:76:PRO:HD2	1.97	0.79
1:E:75:LEU:N	1:E:76:PRO:HD2	1.98	0.79
1:E:258:ARG:HH22	1:E:265:ASP:HB2	1.48	0.78
1:B:174:ASN:OD1	1:B:174:ASN:N	2.17	0.78
1:A:317:LEU:HD21	1:A:380:LEU:HD21	1.66	0.77
1:F:157:ILE:HG13	1:F:158:ASP:N	1.99	0.77
1:C:356:GLN:NE2	1:D:379:GLN:OE1	2.16	0.77
1:F:193:LYS:O	1:F:350:VAL:HG22	1.84	0.77
1:B:52:MET:HG3	1:B:62:VAL:CG1	2.15	0.77
1:D:124:VAL:HG12	1:E:110:LYS:HG3	1.67	0.76
1:C:229:HIS:HD2	1:C:289:GLN:OE1	1.67	0.75
1:A:190:TYR:OH	1:F:256:ALA:CB	2.33	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:MET:HG3	1:A:62:VAL:CG1	2.15	0.75
1:E:229:HIS:HD2	1:E:289:GLN:OE1	1.70	0.74
1:B:392:ARG:HG3	1:B:406:VAL:HG22	1.67	0.74
1:B:36:THR:H	1:B:39:HIS:CD2	2.06	0.74
1:F:229:HIS:HD2	1:F:289:GLN:OE1	1.70	0.73
1:C:175:ILE:HD12	1:C:175:ILE:H	1.51	0.73
1:E:168:ILE:CG1	1:E:169:GLU:H	1.95	0.73
1:D:75:LEU:N	1:D:76:PRO:HD2	2.03	0.73
1:F:52:MET:HG3	1:F:62:VAL:CG1	2.18	0.73
1:B:256:ALA:O	1:C:171:ALA:HB1	1.89	0.72
1:E:273:ILE:HG23	1:F:165:TYR:CE2	2.24	0.72
1:B:193:LYS:O	1:B:350:VAL:HG22	1.89	0.72
1:F:158:ASP:OD1	1:F:161:LEU:HD13	1.89	0.72
1:F:406:VAL:HG23	1:F:425:PHE:HB2	1.72	0.72
1:F:75:LEU:N	1:F:76:PRO:HD2	2.05	0.72
1:A:392:ARG:HG3	1:A:406:VAL:HG22	1.69	0.72
1:D:259:ARG:HG2	1:E:171:ALA:HB2	1.71	0.72
1:E:52:MET:CG	1:E:62:VAL:HG11	2.19	0.72
1:D:107:TYR:O	1:D:111:ARG:HG3	1.90	0.72
1:E:392:ARG:HG3	1:E:406:VAL:HG22	1.71	0.72
1:A:22:SER:N	1:A:91:VAL:HG21	2.05	0.72
1:A:229:HIS:HD2	1:A:289:GLN:OE1	1.73	0.71
1:A:193:LYS:O	1:A:350:VAL:HG22	1.89	0.71
1:A:52:MET:CG	1:A:62:VAL:HG11	2.20	0.71
1:D:193:LYS:O	1:D:350:VAL:HG22	1.90	0.71
1:B:231:LEU:H	1:B:231:LEU:HD12	1.56	0.71
1:E:193:LYS:O	1:E:350:VAL:HG22	1.91	0.71
1:A:333:ILE:HG21	1:A:377:SER:HB3	1.73	0.71
1:B:110:LYS:HG3	1:C:124:VAL:HG11	1.71	0.71
1:C:75:LEU:N	1:C:76:PRO:HD2	2.05	0.70
1:C:193:LYS:O	1:C:350:VAL:HG22	1.92	0.70
1:C:52:MET:HG3	1:C:62:VAL:CG1	2.19	0.70
1:A:254:ILE:HG13	1:B:168:ILE:HD12	1.73	0.70
1:C:392:ARG:HG3	1:C:406:VAL:HG22	1.73	0.69
1:C:281:ILE:O	1:D:157:ILE:HG23	1.91	0.69
1:B:75:LEU:N	1:B:76:PRO:HD2	2.08	0.69
1:E:232:GLU:CD	1:F:414:ARG:HD3	2.11	0.69
1:D:229:HIS:HD2	1:D:289:GLN:OE1	1.75	0.69
1:A:231:LEU:H	1:A:231:LEU:HD12	1.58	0.68
1:F:107:TYR:O	1:F:111:ARG:HG3	1.93	0.68
1:E:239:ILE:HD11	1:F:161:LEU:HG	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:GLU:O	1:A:28:GLU:N	2.26	0.68
1:B:124:VAL:HG11	1:C:110:LYS:HG3	1.74	0.68
1:D:124:VAL:CG1	1:E:110:LYS:HG3	2.23	0.68
1:B:362:GLU:HB2	1:C:372:SER:HB3	1.76	0.68
1:E:158:ASP:O	1:E:160:ALA:N	2.24	0.67
1:E:377:SER:HB2	1:E:380:LEU:CB	2.24	0.67
1:C:119:GLN:HG3	1:C:123:ASN:ND2	2.10	0.67
1:D:392:ARG:HG3	1:D:406:VAL:HG22	1.74	0.67
1:A:157:ILE:CG2	1:A:158:ASP:H	2.07	0.67
1:E:231:LEU:H	1:E:231:LEU:HD12	1.60	0.67
1:F:315:ASP:O	1:F:316:TYR:CB	2.41	0.67
1:E:392:ARG:CG	1:E:406:VAL:HG22	2.25	0.66
1:A:377:SER:HB2	1:A:380:LEU:CB	2.25	0.66
1:A:406:VAL:HG23	1:A:425:PHE:HB2	1.76	0.66
1:C:231:LEU:HD12	1:C:231:LEU:H	1.60	0.66
1:D:377:SER:HB2	1:D:380:LEU:CB	2.26	0.66
1:F:231:LEU:H	1:F:231:LEU:HD12	1.61	0.66
1:C:315:ASP:O	1:C:316:TYR:CB	2.41	0.66
1:B:406:VAL:HG23	1:B:425:PHE:HB2	1.78	0.66
1:C:258:ARG:HG2	1:D:168:ILE:HG22	1.78	0.65
1:B:48:ILE:O	1:B:52:MET:HB2	1.97	0.65
1:D:406:VAL:HG23	1:D:425:PHE:HB2	1.77	0.65
1:D:52:MET:CG	1:D:62:VAL:HG11	2.17	0.65
1:E:48:ILE:O	1:E:52:MET:HB2	1.96	0.65
1:A:124:VAL:HG11	1:F:110:LYS:HG3	1.79	0.65
1:A:161:LEU:HD11	1:F:273:ILE:HG23	1.78	0.65
1:F:124:VAL:HG13	1:F:134:PRO:HB3	1.78	0.65
1:E:23:ILE:HG21	1:E:30:ILE:HG23	1.79	0.65
1:B:119:GLN:HG3	1:B:123:ASN:ND2	2.11	0.64
1:A:36:THR:H	1:A:39:HIS:CD2	2.14	0.64
1:E:315:ASP:O	1:E:316:TYR:CB	2.41	0.64
1:E:273:ILE:HG23	1:F:165:TYR:HE2	1.60	0.64
1:F:392:ARG:HG3	1:F:406:VAL:HG22	1.79	0.64
1:C:392:ARG:CG	1:C:406:VAL:HG22	2.28	0.64
1:B:167:GLU:O	1:B:171:ALA:HB2	1.96	0.64
1:C:406:VAL:HG23	1:C:425:PHE:HB2	1.77	0.64
1:F:257:ALA:HB1	1:F:261:PHE:CB	2.27	0.64
1:F:377:SER:HB2	1:F:380:LEU:CB	2.27	0.64
1:E:406:VAL:HG23	1:E:425:PHE:HB2	1.79	0.64
1:D:392:ARG:CG	1:D:406:VAL:HG22	2.28	0.64
1:D:273:ILE:CG2	1:E:161:LEU:HD11	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:119:GLN:HG3	1:F:123:ASN:ND2	2.12	0.64
1:A:137:GLU:O	1:A:141:GLU:HG2	1.98	0.63
1:F:36:THR:H	1:F:39:HIS:CD2	2.15	0.63
1:A:315:ASP:O	1:A:316:TYR:CB	2.40	0.62
1:B:175:ILE:H	1:B:175:ILE:HD12	1.64	0.62
1:B:107:TYR:O	1:B:111:ARG:HG3	2.00	0.62
1:D:119:GLN:HG3	1:D:123:ASN:ND2	2.15	0.62
1:B:124:VAL:HG13	1:B:134:PRO:HB3	1.82	0.62
1:C:356:GLN:HE22	1:D:379:GLN:CD	2.02	0.62
1:A:154:ASP:HB3	1:F:300:GLN:HE22	1.65	0.61
1:D:333:ILE:HG21	1:D:377:SER:HB3	1.82	0.61
1:F:316:TYR:HB3	1:F:319:LEU:HB2	1.81	0.61
1:C:258:ARG:HG2	1:D:168:ILE:HG23	1.81	0.61
1:E:333:ILE:HG21	1:E:377:SER:HB3	1.81	0.61
1:C:137:GLU:O	1:C:141:GLU:HG2	2.00	0.61
1:B:229:HIS:HD2	1:B:289:GLN:OE1	1.83	0.61
1:C:174:ASN:O	1:C:175:ILE:C	2.39	0.61
1:A:110:LYS:HG3	1:F:124:VAL:HG11	1.82	0.61
1:C:36:THR:H	1:C:39:HIS:CD2	2.18	0.61
1:F:333:ILE:HG21	1:F:377:SER:HB3	1.83	0.61
1:F:157:ILE:CG1	1:F:158:ASP:N	2.63	0.61
1:A:37:PRO:HB2	1:A:46:PHE:CE1	2.36	0.60
1:D:375:ARG:HE	1:D:376:GLU:HG3	1.65	0.60
1:D:36:THR:H	1:D:39:HIS:CD2	2.18	0.60
1:D:231:LEU:HD12	1:D:231:LEU:H	1.65	0.60
1:C:107:TYR:O	1:C:111:ARG:HG3	2.01	0.60
1:D:257:ALA:HB1	1:D:261:PHE:CB	2.31	0.60
1:B:259:ARG:H	1:C:171:ALA:HB3	1.66	0.60
1:C:317:LEU:CD2	1:C:380:LEU:HD21	2.29	0.60
1:C:203:ARG:NH2	1:D:381:GLU:OE1	2.32	0.60
1:E:255:LYS:HG2	1:F:190:TYR:CD1	2.37	0.60
1:A:26:GLU:C	1:A:28:GLU:H	2.04	0.60
1:A:190:TYR:HH	1:F:256:ALA:HB2	1.67	0.59
1:A:124:VAL:HG13	1:A:134:PRO:HB3	1.83	0.59
1:A:157:ILE:CG2	1:A:158:ASP:N	2.65	0.59
1:A:48:ILE:O	1:A:52:MET:HB2	2.02	0.59
1:B:392:ARG:CG	1:B:406:VAL:HG22	2.33	0.59
1:B:52:MET:CG	1:B:62:VAL:HG11	2.27	0.59
1:D:357:LEU:HD13	1:D:369:PRO:HB3	1.85	0.59
1:B:154:ASP:OD1	1:B:155:GLY:N	2.34	0.59
1:A:164:VAL:O	1:A:168:ILE:HG12	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:377:SER:HB2	1:B:380:LEU:CB	2.30	0.59
1:C:48:ILE:O	1:C:52:MET:HB2	2.03	0.59
1:F:41:SER:HB3	1:F:42:PRO:HD2	1.84	0.59
1:C:172:ASP:O	1:C:174:ASN:N	2.35	0.59
1:A:119:GLN:HG3	1:A:123:ASN:ND2	2.18	0.58
1:A:357:LEU:HD13	1:A:369:PRO:HB3	1.85	0.58
1:B:333:ILE:HG21	1:B:377:SER:HB3	1.84	0.58
1:C:356:GLN:CD	1:D:382:GLN:OE1	2.42	0.58
1:D:98:LYS:HE2	1:D:98:LYS:HA	1.84	0.58
1:E:317:LEU:CD2	1:E:380:LEU:HD21	2.32	0.58
1:B:316:TYR:HB3	1:B:319:LEU:HB2	1.85	0.58
1:C:377:SER:HB2	1:C:380:LEU:CB	2.28	0.58
1:C:257:ALA:HB1	1:C:261:PHE:CB	2.34	0.57
1:A:75:LEU:N	1:A:76:PRO:CD	2.67	0.57
1:E:12:ASN:HD21	1:F:69:ALA:HA	1.69	0.57
1:C:254:ILE:HA	1:C:258:ARG:HB2	1.86	0.57
1:B:305:ASN:HB3	1:B:308:LYS:HD2	1.85	0.57
1:C:333:ILE:HG21	1:C:377:SER:HB3	1.85	0.57
1:F:317:LEU:CD2	1:F:380:LEU:HD21	2.30	0.57
1:A:316:TYR:HB3	1:A:319:LEU:HB2	1.87	0.57
1:F:392:ARG:CG	1:F:406:VAL:HG22	2.33	0.57
1:B:22:SER:N	1:B:91:VAL:HG21	2.19	0.57
1:E:36:THR:H	1:E:39:HIS:CD2	2.22	0.57
1:C:316:TYR:HB3	1:C:319:LEU:HB2	1.87	0.57
1:C:16:GLU:OE2	1:C:40:PHE:HA	2.05	0.57
1:D:316:TYR:HB3	1:D:319:LEU:HB2	1.87	0.57
1:D:22:SER:N	1:D:91:VAL:HG21	2.19	0.57
1:A:258:ARG:CG	1:B:168:ILE:HG23	2.32	0.57
1:B:37:PRO:HB2	1:B:46:PHE:CE1	2.39	0.57
1:E:254:ILE:HA	1:E:258:ARG:HB2	1.85	0.57
1:D:48:ILE:O	1:D:52:MET:HB2	2.04	0.56
1:B:124:VAL:CG1	1:C:110:LYS:HG3	2.35	0.56
1:F:375:ARG:HE	1:F:376:GLU:HG3	1.70	0.56
1:A:236:LYS:NZ	1:B:163:THR:HG21	2.20	0.56
1:B:375:ARG:HE	1:B:376:GLU:HG3	1.71	0.56
1:D:305:ASN:HB3	1:D:308:LYS:HD2	1.88	0.56
1:C:22:SER:N	1:C:91:VAL:HG21	2.20	0.56
1:F:254:ILE:HG23	1:F:255:LYS:H	1.71	0.56
1:A:254:ILE:HA	1:A:258:ARG:HB2	1.88	0.56
1:A:254:ILE:HG13	1:B:168:ILE:CD1	2.34	0.56
1:C:299:ARG:NH1	1:C:299:ARG:HB3	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:119:GLN:HG3	1:E:123:ASN:ND2	2.20	0.56
1:C:299:ARG:NH1	1:D:31:LYS:O	2.39	0.56
1:F:378:GLY:C	1:F:380:LEU:H	2.09	0.56
1:C:375:ARG:HE	1:C:376:GLU:HG3	1.71	0.56
1:E:357:LEU:HD13	1:E:369:PRO:HB3	1.87	0.56
1:A:364:ARG:HD2	1:F:359:ARG:CZ	2.35	0.55
1:E:316:TYR:HB3	1:E:319:LEU:HB2	1.87	0.55
1:B:157:ILE:O	1:B:161:LEU:N	2.34	0.55
1:E:158:ASP:C	1:E:160:ALA:H	2.08	0.55
1:E:305:ASN:HB3	1:E:308:LYS:HD2	1.89	0.55
1:B:315:ASP:O	1:B:316:TYR:CB	2.41	0.55
1:B:257:ALA:HB1	1:B:261:PHE:CB	2.36	0.55
1:C:282:ASN:HA	1:D:157:ILE:HG23	1.89	0.55
1:F:254:ILE:O	1:F:255:LYS:C	2.44	0.55
1:B:254:ILE:HA	1:B:258:ARG:HB2	1.89	0.55
1:D:317:LEU:CD2	1:D:380:LEU:HD21	2.35	0.55
1:B:165:TYR:O	1:B:168:ILE:N	2.36	0.55
1:B:254:ILE:HG13	1:C:168:ILE:HG23	1.89	0.55
1:C:357:LEU:HD13	1:C:369:PRO:HB3	1.88	0.55
1:D:424:ALA:HB3	1:D:433:VAL:HB	1.89	0.54
1:A:392:ARG:CG	1:A:406:VAL:HG22	2.36	0.54
1:A:254:ILE:HG23	1:A:255:LYS:H	1.72	0.54
1:A:254:ILE:O	1:A:255:LYS:C	2.46	0.54
1:B:317:LEU:CD2	1:B:380:LEU:HD21	2.35	0.54
1:A:375:ARG:HE	1:A:376:GLU:HG3	1.72	0.54
1:A:392:ARG:HH21	1:A:427:LYS:HE2	1.73	0.54
1:D:254:ILE:HG23	1:D:255:LYS:H	1.73	0.54
1:B:165:TYR:O	1:B:168:ILE:HG12	2.08	0.54
1:D:315:ASP:O	1:D:316:TYR:CB	2.42	0.54
1:E:99:GLN:HE22	1:F:61:SER:H	1.54	0.54
1:F:23:ILE:HG21	1:F:30:ILE:HG23	1.89	0.54
1:E:75:LEU:N	1:E:76:PRO:CD	2.69	0.54
1:F:357:LEU:HD13	1:F:369:PRO:HB3	1.90	0.54
1:F:37:PRO:HB2	1:F:46:PHE:CE1	2.42	0.54
1:C:172:ASP:C	1:C:174:ASN:H	2.09	0.54
1:B:229:HIS:CD2	1:B:294:ILE:HG12	2.43	0.54
1:F:48:ILE:O	1:F:52:MET:HB2	2.08	0.54
1:D:201:ALA:O	1:D:389:PHE:HA	2.07	0.54
1:E:162:VAL:O	1:E:165:TYR:HB2	2.08	0.53
1:E:424:ALA:HB3	1:E:433:VAL:HB	1.90	0.53
1:C:52:MET:CG	1:C:62:VAL:HG11	2.28	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:23:ILE:HG21	1:D:30:ILE:HG23	1.89	0.53
1:B:357:LEU:HD13	1:B:369:PRO:HB3	1.90	0.53
1:C:392:ARG:HH21	1:C:427:LYS:HE2	1.72	0.53
1:A:138:ALA:O	1:A:142:LEU:HB2	2.08	0.53
1:C:96:THR:HG22	1:D:61:SER:OG	2.09	0.53
1:A:317:LEU:CD2	1:A:380:LEU:HD21	2.36	0.53
1:F:137:GLU:O	1:F:141:GLU:HG2	2.09	0.53
1:F:316:TYR:HD2	1:F:319:LEU:HD13	1.73	0.53
1:A:424:ALA:HB3	1:A:433:VAL:HB	1.91	0.53
1:A:27:PRO:HB3	1:A:62:VAL:O	2.08	0.53
1:C:378:GLY:C	1:C:380:LEU:H	2.12	0.53
1:E:107:TYR:O	1:E:111:ARG:HG3	2.08	0.53
1:A:378:GLY:C	1:A:380:LEU:H	2.11	0.53
1:A:257:ALA:HB1	1:A:261:PHE:CB	2.39	0.53
1:D:161:LEU:O	1:D:161:LEU:HD23	2.08	0.53
1:B:392:ARG:HH21	1:B:427:LYS:HE2	1.72	0.53
1:E:257:ALA:HB1	1:E:261:PHE:CB	2.39	0.53
1:C:305:ASN:HB3	1:C:308:LYS:HD2	1.90	0.53
1:D:254:ILE:O	1:D:255:LYS:C	2.47	0.53
1:F:305:ASN:HB3	1:F:308:LYS:HD2	1.91	0.53
1:B:316:TYR:HD2	1:B:319:LEU:HD13	1.74	0.52
1:D:378:GLY:C	1:D:380:LEU:H	2.12	0.52
1:E:282:ASN:HA	1:F:157:ILE:HB	1.89	0.52
1:A:99:GLN:HE22	1:B:61:SER:H	1.57	0.52
1:B:165:TYR:O	1:B:166:GLU:C	2.47	0.52
1:F:52:MET:CG	1:F:62:VAL:HG11	2.24	0.52
1:B:156:SER:C	1:B:157:ILE:HG13	2.29	0.52
1:C:115:SER:O	1:C:119:GLN:HB2	2.09	0.52
1:F:150:THR:O	1:F:151:ASP:HB3	2.09	0.52
1:A:41:SER:HB3	1:A:42:PRO:HD2	1.91	0.52
1:A:160:ALA:O	1:A:164:VAL:HG23	2.10	0.52
1:B:201:ALA:O	1:B:389:PHE:HA	2.10	0.52
1:B:259:ARG:NH1	1:C:169:GLU:HG2	2.24	0.52
1:D:157:ILE:HG13	1:D:157:ILE:O	2.09	0.52
1:E:392:ARG:HH21	1:E:427:LYS:HE2	1.74	0.52
1:F:123:ASN:HB3	1:F:137:GLU:OE1	2.09	0.52
1:B:254:ILE:O	1:B:255:LYS:C	2.48	0.52
1:A:362:GLU:HB2	1:B:372:SER:HB3	1.91	0.52
1:C:41:SER:HB3	1:C:42:PRO:HD2	1.91	0.52
1:F:392:ARG:HH21	1:F:427:LYS:HE2	1.73	0.52
1:C:232:GLU:HG3	1:D:341:LYS:HE2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:115:SER:O	1:E:119:GLN:HB2	2.09	0.52
1:F:16:GLU:OE2	1:F:40:PHE:HA	2.10	0.52
1:A:93:SER:C	1:A:95:THR:H	2.14	0.51
1:C:175:ILE:HD12	1:C:175:ILE:N	2.21	0.51
1:C:254:ILE:O	1:C:255:LYS:C	2.48	0.51
1:D:392:ARG:HH21	1:D:427:LYS:HE2	1.75	0.51
1:E:316:TYR:HD2	1:E:319:LEU:HD13	1.75	0.51
1:B:64:PHE:N	1:B:64:PHE:CD1	2.78	0.51
1:E:254:ILE:O	1:E:255:LYS:C	2.49	0.51
1:A:305:ASN:HB3	1:A:308:LYS:HD2	1.93	0.51
1:B:26:GLU:C	1:B:28:GLU:H	2.14	0.51
1:B:134:PRO:HG3	1:C:110:LYS:HB2	1.92	0.51
1:E:386:ILE:HA	1:E:412:LYS:O	2.10	0.51
1:A:16:GLU:OE2	1:A:40:PHE:HA	2.11	0.51
1:C:23:ILE:HG21	1:C:30:ILE:HG23	1.92	0.51
1:D:254:ILE:HA	1:D:258:ARG:HB2	1.93	0.51
1:B:254:ILE:HG23	1:B:255:LYS:H	1.76	0.51
1:C:356:GLN:OE1	1:D:382:GLN:OE1	2.29	0.51
1:D:141:GLU:O	1:D:145:ILE:HG13	2.11	0.51
1:A:198:VAL:HG22	1:A:352:ILE:HG12	1.92	0.51
1:A:123:ASN:HB3	1:A:137:GLU:OE1	2.11	0.51
1:A:169:GLU:HB2	1:F:259:ARG:NH1	2.26	0.50
1:A:316:TYR:HD2	1:A:319:LEU:HD13	1.76	0.50
1:B:378:GLY:C	1:B:380:LEU:H	2.14	0.50
1:D:16:GLU:OE2	1:D:40:PHE:HA	2.11	0.50
1:D:75:LEU:N	1:D:76:PRO:CD	2.73	0.50
1:F:167:GLU:OE1	1:F:167:GLU:N	2.40	0.50
1:F:198:VAL:HG22	1:F:352:ILE:HG12	1.93	0.50
1:A:371:LEU:HD11	1:A:411:ALA:HB1	1.94	0.50
1:B:435:LEU:O	1:B:436:GLU:HB2	2.11	0.50
1:E:375:ARG:HE	1:E:376:GLU:HG3	1.75	0.50
1:A:146:GLU:C	1:A:148:SER:H	2.14	0.50
1:A:175:ILE:N	1:A:175:ILE:HD12	2.26	0.50
1:E:208:LYS:HD2	1:E:355:SER:O	2.11	0.50
1:E:254:ILE:HD11	1:F:168:ILE:HD12	1.94	0.50
1:B:110:LYS:HG3	1:C:124:VAL:CG1	2.41	0.50
1:A:115:SER:O	1:A:119:GLN:HB2	2.11	0.50
1:A:256:ALA:O	1:B:171:ALA:HB1	2.11	0.50
1:B:23:ILE:HG21	1:B:30:ILE:HG23	1.93	0.50
1:A:157:ILE:HD13	1:A:158:ASP:N	2.27	0.50
1:C:424:ALA:HB3	1:C:433:VAL:HB	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:75:LEU:N	1:C:76:PRO:CD	2.74	0.50
1:D:157:ILE:CG1	1:D:157:ILE:O	2.59	0.50
1:E:22:SER:N	1:E:91:VAL:HG21	2.26	0.49
1:E:378:GLY:C	1:E:380:LEU:H	2.14	0.49
1:A:364:ARG:HD2	1:F:359:ARG:NH2	2.27	0.49
1:B:115:SER:O	1:B:119:GLN:HB2	2.12	0.49
1:B:137:GLU:O	1:B:141:GLU:HG2	2.13	0.49
1:D:358:SER:HB2	1:D:375:ARG:HB2	1.94	0.49
1:C:303:ARG:NH1	1:D:98:LYS:HD2	2.27	0.49
1:D:316:TYR:HD2	1:D:319:LEU:HD13	1.78	0.49
1:F:75:LEU:N	1:F:76:PRO:CD	2.75	0.49
1:C:198:VAL:HG22	1:C:352:ILE:HG12	1.94	0.49
1:F:138:ALA:O	1:F:142:LEU:HB2	2.13	0.49
1:E:167:GLU:HA	1:E:170:SER:HB2	1.94	0.49
1:B:120:ILE:HG23	1:B:141:GLU:HG3	1.95	0.49
1:F:161:LEU:O	1:F:164:VAL:HG22	2.13	0.49
1:B:16:GLU:OE2	1:B:40:PHE:HA	2.12	0.48
1:F:41:SER:O	1:F:46:PHE:HB2	2.12	0.48
1:A:141:GLU:O	1:A:145:ILE:HG13	2.12	0.48
1:B:119:GLN:HG3	1:B:123:ASN:HD22	1.77	0.48
1:D:20:LEU:O	1:D:24:LEU:HG	2.14	0.48
1:F:280:ASN:HD22	1:F:280:ASN:N	2.11	0.48
1:F:64:PHE:CD1	1:F:64:PHE:N	2.82	0.48
1:F:22:SER:N	1:F:91:VAL:HG21	2.28	0.48
1:B:239:ILE:HG21	1:C:161:LEU:HG	1.96	0.48
1:D:338:ARG:HG3	1:D:379:GLN:HG2	1.95	0.48
1:F:217:LYS:O	1:F:220:SER:N	2.47	0.48
1:C:120:ILE:O	1:C:124:VAL:HG23	2.14	0.48
1:B:258:ARG:HB3	1:C:171:ALA:CB	2.44	0.48
1:B:386:ILE:HA	1:B:412:LYS:O	2.14	0.48
1:E:142:LEU:O	1:E:146:GLU:HG3	2.14	0.48
1:E:337:SER:HB2	1:E:380:LEU:HD22	1.95	0.48
1:D:359:ARG:NH1	1:E:366:ASP:HB3	2.29	0.48
1:F:406:VAL:HG23	1:F:425:PHE:CB	2.42	0.48
1:A:356:GLN:HE22	1:B:382:GLN:CD	2.17	0.48
1:B:362:GLU:HB2	1:C:372:SER:CB	2.41	0.48
1:F:125:ASN:OD1	1:F:125:ASN:N	2.46	0.48
1:F:337:SER:HB2	1:F:380:LEU:HD22	1.96	0.48
1:B:116:ILE:HG12	1:B:144:GLU:HB3	1.95	0.47
1:E:282:ASN:ND2	1:F:157:ILE:HD13	2.29	0.47
1:A:157:ILE:HD13	1:A:158:ASP:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:142:LEU:O	1:C:146:GLU:HG3	2.14	0.47
1:D:26:GLU:C	1:D:28:GLU:H	2.17	0.47
1:E:239:ILE:HD11	1:F:161:LEU:CG	2.43	0.47
1:A:414:ARG:O	1:F:237:GLU:OE1	2.32	0.47
1:A:31:LYS:HE3	1:A:56:ASP:OD1	2.14	0.47
1:B:175:ILE:HD12	1:B:175:ILE:N	2.28	0.47
1:E:241:ARG:HH21	1:F:415:ASP:HA	1.79	0.47
1:F:424:ALA:HB3	1:F:433:VAL:HB	1.95	0.47
1:A:313:MET:HA	1:A:352:ILE:O	2.14	0.47
1:A:386:ILE:HA	1:A:412:LYS:O	2.15	0.47
1:B:337:SER:HB2	1:B:380:LEU:HD22	1.95	0.47
1:C:26:GLU:C	1:C:28:GLU:H	2.18	0.47
1:F:257:ALA:O	1:F:259:ARG:N	2.48	0.47
1:E:316:TYR:CD2	1:E:319:LEU:HD13	2.49	0.47
1:F:358:SER:HB2	1:F:375:ARG:HB2	1.95	0.47
1:A:229:HIS:CD2	1:A:294:ILE:HG12	2.50	0.47
1:E:282:ASN:ND2	1:F:157:ILE:CD1	2.78	0.47
1:D:316:TYR:CD2	1:D:319:LEU:HD13	2.49	0.47
1:A:269:LEU:C	1:A:271:MET:H	2.17	0.47
1:F:254:ILE:HA	1:F:258:ARG:HB2	1.97	0.47
1:A:152:ASP:N	1:A:152:ASP:OD1	2.48	0.46
1:B:316:TYR:CD2	1:B:319:LEU:HD13	2.50	0.46
1:A:142:LEU:O	1:A:146:GLU:HG3	2.14	0.46
1:B:138:ALA:O	1:B:142:LEU:HB2	2.15	0.46
1:E:160:ALA:O	1:E:164:VAL:N	2.42	0.46
1:C:201:ALA:O	1:C:389:PHE:HA	2.16	0.46
1:C:410:ILE:HD12	1:C:410:ILE:N	2.31	0.46
1:B:75:LEU:N	1:B:76:PRO:CD	2.76	0.46
1:C:358:SER:HB2	1:C:375:ARG:HB2	1.98	0.46
1:E:44:LYS:O	1:E:48:ILE:HG12	2.15	0.46
1:B:368:ARG:HA	1:B:369:PRO:HD3	1.77	0.46
1:C:99:GLN:HE22	1:D:61:SER:H	1.64	0.46
1:E:157:ILE:CG1	1:E:158:ASP:N	2.70	0.46
1:F:174:ASN:O	1:F:175:ILE:O	2.34	0.46
1:A:217:LYS:O	1:A:220:SER:N	2.49	0.46
1:A:259:ARG:HB3	1:B:171:ALA:O	2.16	0.46
1:F:254:ILE:O	1:F:258:ARG:HB2	2.16	0.46
1:F:316:TYR:CD2	1:F:319:LEU:HD13	2.50	0.46
1:A:64:PHE:N	1:A:64:PHE:CD1	2.84	0.46
1:C:41:SER:O	1:C:46:PHE:HB2	2.16	0.46
1:D:406:VAL:HG23	1:D:425:PHE:CB	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:362:GLU:HB2	1:F:372:SER:HB3	1.97	0.46
1:E:406:VAL:HG23	1:E:425:PHE:CB	2.45	0.46
1:A:239:ILE:HD13	1:B:161:LEU:HD22	1.97	0.46
1:E:137:GLU:O	1:E:141:GLU:HG2	2.16	0.45
1:E:368:ARG:HA	1:E:369:PRO:HD3	1.79	0.45
1:F:257:ALA:HB1	1:F:261:PHE:HB2	1.98	0.45
1:A:12:ASN:HD21	1:B:69:ALA:HA	1.81	0.45
1:E:229:HIS:CD2	1:E:294:ILE:HG12	2.52	0.45
1:B:258:ARG:HB3	1:C:171:ALA:HB2	1.97	0.45
1:C:254:ILE:HG23	1:C:255:LYS:H	1.81	0.45
1:E:254:ILE:HG23	1:E:255:LYS:H	1.81	0.45
1:A:203:ARG:NH1	1:A:359:ARG:HA	2.31	0.45
1:C:208:LYS:HD2	1:C:355:SER:O	2.17	0.45
1:D:41:SER:HB3	1:D:42:PRO:HD2	1.98	0.45
1:B:175:ILE:H	1:B:175:ILE:CD1	2.29	0.45
1:B:406:VAL:HG23	1:B:425:PHE:CB	2.45	0.45
1:E:169:GLU:O	1:E:170:SER:O	2.35	0.45
1:E:172:ASP:N	1:E:172:ASP:OD2	2.50	0.45
1:E:381:GLU:HA	1:E:387:ILE:HD11	1.98	0.45
1:C:299:ARG:HB3	1:C:299:ARG:HH11	1.82	0.45
1:D:435:LEU:O	1:D:436:GLU:C	2.55	0.45
1:E:356:GLN:OE1	1:F:382:GLN:HG2	2.17	0.45
1:C:406:VAL:HG23	1:C:425:PHE:CB	2.45	0.45
1:E:175:ILE:N	1:E:175:ILE:HD12	2.31	0.45
1:E:254:ILE:O	1:E:258:ARG:HB2	2.16	0.45
1:E:26:GLU:C	1:E:28:GLU:H	2.20	0.45
1:F:254:ILE:HA	1:F:258:ARG:HD2	1.99	0.45
1:F:406:VAL:CG2	1:F:425:PHE:HB2	2.44	0.45
1:C:367:LYS:HB2	1:C:391:TYR:HE1	1.82	0.44
1:F:212:ALA:HB1	1:F:313:MET:CE	2.46	0.44
1:F:257:ALA:O	1:F:258:ARG:C	2.55	0.44
1:D:119:GLN:HG3	1:D:123:ASN:HD22	1.81	0.44
1:E:138:ALA:O	1:E:142:LEU:HB2	2.17	0.44
1:A:39:HIS:HE1	1:A:151:ASP:OD2	2.01	0.44
1:A:152:ASP:HB2	1:A:153:ASP:H	1.52	0.44
1:A:357:LEU:CD1	1:A:369:PRO:HB3	2.46	0.44
1:A:236:LYS:HZ1	1:B:163:THR:HG21	1.82	0.44
1:D:386:ILE:HA	1:D:412:LYS:O	2.18	0.44
1:D:237:GLU:CD	1:E:415:ASP:HA	2.37	0.44
1:A:316:TYR:CD2	1:A:319:LEU:HD13	2.53	0.44
1:E:280:ASN:HD22	1:E:280:ASN:N	2.14	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:201:ALA:O	1:F:202:ALA:HB2	2.17	0.44
1:B:371:LEU:HD11	1:B:411:ALA:HB1	2.00	0.44
1:B:258:ARG:HG2	1:C:168:ILE:O	2.16	0.44
1:C:37:PRO:HB2	1:C:46:PHE:CE1	2.52	0.44
1:D:368:ARG:HA	1:D:369:PRO:HD3	1.81	0.44
1:D:44:LYS:O	1:D:48:ILE:HG12	2.17	0.44
1:A:201:ALA:O	1:A:389:PHE:HA	2.17	0.44
1:A:212:ALA:HB2	1:A:354:LEU:HD11	2.00	0.44
1:A:337:SER:HB2	1:A:380:LEU:HD22	1.99	0.44
1:E:282:ASN:HD21	1:F:157:ILE:HD13	1.82	0.44
1:F:410:ILE:N	1:F:410:ILE:HD12	2.33	0.44
1:F:44:LYS:O	1:F:48:ILE:HG12	2.18	0.44
1:D:410:ILE:N	1:D:410:ILE:HD12	2.33	0.44
1:A:212:ALA:HB1	1:A:313:MET:CE	2.48	0.44
1:E:171:ALA:O	1:E:172:ASP:HB3	2.17	0.44
1:C:280:ASN:N	1:C:280:ASN:HD22	2.16	0.43
1:D:124:VAL:HG13	1:D:134:PRO:HB3	2.00	0.43
1:E:201:ALA:O	1:E:389:PHE:HA	2.17	0.43
1:F:201:ALA:O	1:F:389:PHE:HA	2.19	0.43
1:A:154:ASP:CB	1:F:300:GLN:HE22	2.30	0.43
1:A:178:VAL:O	1:A:191:GLY:HA2	2.18	0.43
1:A:30:ILE:HD12	1:A:31:LYS:H	1.83	0.43
1:A:406:VAL:CG2	1:A:425:PHE:HB2	2.47	0.43
1:F:161:LEU:HD23	1:F:161:LEU:O	2.18	0.43
1:A:259:ARG:CB	1:B:171:ALA:O	2.67	0.43
1:C:254:ILE:HA	1:C:258:ARG:HD2	2.00	0.43
1:F:146:GLU:C	1:F:148:SER:H	2.22	0.43
1:B:259:ARG:HB2	1:C:171:ALA:H	1.83	0.43
1:A:406:VAL:HG23	1:A:425:PHE:CB	2.44	0.43
1:B:165:TYR:O	1:B:167:GLU:N	2.52	0.43
1:E:410:ILE:N	1:E:410:ILE:HD12	2.33	0.43
1:D:254:ILE:O	1:D:258:ARG:HB2	2.19	0.43
1:F:158:ASP:HA	1:F:161:LEU:HB3	2.00	0.43
1:C:368:ARG:HA	1:C:369:PRO:HD3	1.79	0.43
1:D:311:ILE:HG13	1:D:350:VAL:HB	2.00	0.43
1:F:157:ILE:HG13	1:F:158:ASP:OD1	2.18	0.43
1:A:338:ARG:HG3	1:A:379:GLN:HG2	2.00	0.43
1:B:256:ALA:HB3	1:C:190:TYR:CE2	2.53	0.43
1:C:254:ILE:O	1:C:258:ARG:HB2	2.19	0.43
1:C:355:SER:OG	1:C:356:GLN:N	2.52	0.43
1:D:64:PHE:CD1	1:D:64:PHE:N	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:ALA:HB1	1:B:313:MET:HE2	2.00	0.42
1:A:198:VAL:CG2	1:A:352:ILE:HG12	2.49	0.42
1:A:254:ILE:O	1:A:258:ARG:HB2	2.19	0.42
1:A:26:GLU:C	1:A:28:GLU:N	2.71	0.42
1:A:358:SER:HB2	1:A:375:ARG:HB2	2.00	0.42
1:C:172:ASP:C	1:C:174:ASN:N	2.72	0.42
1:C:316:TYR:OH	1:D:382:GLN:HB3	2.18	0.42
1:E:161:LEU:O	1:E:164:VAL:HB	2.20	0.42
1:C:262:ALA:HB1	1:C:265:ASP:OD2	2.19	0.42
1:C:337:SER:HB2	1:C:380:LEU:HD22	2.00	0.42
1:D:254:ILE:HA	1:D:258:ARG:HD2	2.00	0.42
1:B:367:LYS:HB2	1:B:391:TYR:HE1	1.85	0.42
1:D:402:SER:HB3	1:D:405:ILE:HB	2.02	0.42
1:E:119:GLN:HG3	1:E:123:ASN:HD22	1.84	0.42
1:E:367:LYS:HB2	1:E:391:TYR:HE1	1.85	0.42
1:F:119:GLN:HG3	1:F:123:ASN:HD22	1.84	0.42
1:A:208:LYS:HD2	1:A:355:SER:O	2.19	0.42
1:C:25:THR:O	1:C:27:PRO:HD3	2.19	0.42
1:D:367:LYS:HB2	1:D:391:TYR:HE1	1.84	0.42
1:A:311:ILE:HD12	1:A:311:ILE:N	2.35	0.42
1:A:52:MET:HG3	1:A:62:VAL:HG13	1.97	0.42
1:E:358:SER:HB2	1:E:375:ARG:HB2	2.01	0.42
1:B:31:LYS:HE3	1:B:56:ASP:OD1	2.20	0.42
1:C:154:ASP:CG	1:C:155:GLY:N	2.72	0.42
1:C:257:ALA:O	1:C:259:ARG:N	2.53	0.42
1:D:145:ILE:O	1:D:145:ILE:HG22	2.20	0.42
1:D:229:HIS:CD2	1:D:294:ILE:HG12	2.54	0.42
1:E:257:ALA:O	1:E:259:ARG:N	2.53	0.42
1:A:171:ALA:O	1:A:172:ASP:C	2.59	0.42
1:A:252:GLN:HG2	1:B:190:TYR:OH	2.19	0.42
1:E:173:GLY:O	1:E:174:ASN:CB	2.66	0.42
1:C:242:LEU:HB3	1:C:276:ILE:HD12	2.01	0.41
1:F:31:LYS:HE3	1:F:56:ASP:OD1	2.20	0.41
1:A:254:ILE:HA	1:A:258:ARG:HD2	2.02	0.41
1:A:292:ASN:HD22	1:B:31:LYS:HD3	1.85	0.41
1:A:381:GLU:HA	1:A:387:ILE:HD11	2.02	0.41
1:D:138:ALA:O	1:D:142:LEU:HB2	2.21	0.41
1:D:49:TYR:HA	1:D:52:MET:HB3	2.02	0.41
1:E:41:SER:O	1:E:46:PHE:HB2	2.20	0.41
1:F:26:GLU:C	1:F:28:GLU:H	2.23	0.41
1:A:212:ALA:HB1	1:A:313:MET:HE2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:386:ILE:HA	1:C:412:LYS:O	2.20	0.41
1:D:406:VAL:CG2	1:D:425:PHE:HB2	2.46	0.41
1:A:269:LEU:C	1:A:271:MET:N	2.74	0.41
1:B:49:TYR:HA	1:B:52:MET:HB3	2.02	0.41
1:C:358:SER:C	1:C:360:GLN:H	2.24	0.41
1:D:115:SER:O	1:D:119:GLN:HB2	2.19	0.41
1:D:198:VAL:HG22	1:D:352:ILE:HG12	2.02	0.41
1:E:198:VAL:HG22	1:E:352:ILE:HG12	2.01	0.41
1:F:269:LEU:C	1:F:271:MET:H	2.23	0.41
1:F:368:ARG:HA	1:F:369:PRO:HD3	1.79	0.41
1:A:311:ILE:HG13	1:A:350:VAL:HB	2.02	0.41
1:C:38:GLU:HG2	1:C:38:GLU:H	1.67	0.41
1:E:167:GLU:O	1:E:170:SER:HB2	2.20	0.41
1:F:26:GLU:HB2	1:F:29:LEU:HD22	2.02	0.41
1:C:138:ALA:O	1:C:142:LEU:HB2	2.20	0.41
1:D:221:ASP:C	1:D:223:ASP:H	2.24	0.41
1:D:25:THR:O	1:D:27:PRO:HD3	2.21	0.41
1:F:163:THR:O	1:F:167:GLU:OE1	2.39	0.41
1:A:150:THR:HG21	1:F:303:ARG:NH2	2.35	0.41
1:A:262:ALA:HB1	1:A:265:ASP:OD2	2.19	0.41
1:A:358:SER:C	1:A:360:GLN:H	2.23	0.41
1:C:49:TYR:HA	1:C:52:MET:HB3	2.03	0.41
1:E:259:ARG:HB2	1:F:171:ALA:O	2.21	0.41
1:C:269:LEU:C	1:C:271:MET:H	2.22	0.41
1:E:201:ALA:O	1:E:202:ALA:HB2	2.20	0.41
1:F:262:ALA:HB1	1:F:265:ASP:OD2	2.20	0.41
1:F:381:GLU:HA	1:F:387:ILE:HD11	2.02	0.41
1:A:12:ASN:O	1:A:16:GLU:HB2	2.21	0.41
1:A:158:ASP:HA	1:A:161:LEU:HB2	2.03	0.41
1:A:201:ALA:O	1:A:202:ALA:HB2	2.20	0.41
1:B:146:GLU:C	1:B:148:SER:H	2.23	0.41
1:B:221:ASP:C	1:B:223:ASP:H	2.24	0.41
1:B:242:LEU:HB3	1:B:276:ILE:HD12	2.03	0.41
1:B:311:ILE:HD12	1:B:311:ILE:N	2.36	0.41
1:E:124:VAL:HG13	1:E:134:PRO:HB3	2.02	0.41
1:F:311:ILE:HD12	1:F:311:ILE:N	2.36	0.41
1:A:178:VAL:HG21	1:A:311:ILE:HD11	2.03	0.41
1:B:215:GLN:O	1:B:219:MET:HG3	2.20	0.41
1:B:410:ILE:HD12	1:B:410:ILE:N	2.36	0.41
1:B:63:ASP:O	1:B:64:PHE:C	2.58	0.41
1:E:326:ASN:HD22	1:E:326:ASN:HA	1.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:LYS:NZ	1:A:308:LYS:HB3	2.36	0.41
1:B:259:ARG:HD3	1:C:169:GLU:O	2.21	0.41
1:C:239:ILE:HD11	1:D:157:ILE:HD12	2.03	0.41
1:C:327:ASP:O	1:D:324:LYS:NZ	2.54	0.41
1:C:338:ARG:HG3	1:C:379:GLN:HG2	2.02	0.41
1:D:344:ALA:HB2	1:D:351:VAL:CG2	2.51	0.41
1:E:313:MET:HA	1:E:352:ILE:O	2.21	0.41
1:E:38:GLU:HG2	1:E:38:GLU:H	1.65	0.41
1:F:212:ALA:HB2	1:F:354:LEU:HD11	2.02	0.41
1:A:158:ASP:C	1:A:160:ALA:N	2.74	0.40
1:A:367:LYS:HB2	1:A:391:TYR:HE1	1.86	0.40
1:C:406:VAL:CG2	1:C:425:PHE:HB2	2.47	0.40
1:D:381:GLU:HA	1:D:387:ILE:HD11	2.03	0.40
1:F:257:ALA:HB1	1:F:261:PHE:HB3	2.02	0.40
1:F:340:LEU:HD23	1:F:340:LEU:HA	1.93	0.40
1:B:313:MET:HA	1:B:352:ILE:O	2.21	0.40
1:B:48:ILE:CD1	1:B:78:LEU:HB3	2.52	0.40
1:D:337:SER:HB2	1:D:380:LEU:HD22	2.03	0.40
1:C:273:ILE:HD13	1:D:165:TYR:CD2	2.57	0.40
1:F:49:TYR:HA	1:F:52:MET:HB3	2.02	0.40
1:C:347:LEU:HD12	1:C:347:LEU:HA	1.89	0.40
1:C:206:MET:CE	1:C:391:TYR:HA	2.52	0.40
1:D:212:ALA:HB2	1:D:354:LEU:HD11	2.04	0.40
1:E:254:ILE:HA	1:E:258:ARG:HD2	2.03	0.40
1:F:244:VAL:HG12	1:F:244:VAL:O	2.20	0.40
1:F:299:ARG:NH1	1:F:299:ARG:HB3	2.37	0.40
1:A:30:ILE:HD12	1:A:31:LYS:N	2.36	0.40
1:B:154:ASP:CG	1:B:155:GLY:N	2.75	0.40
1:B:26:GLU:O	1:B:28:GLU:N	2.50	0.40
1:C:282:ASN:HA	1:D:157:ILE:CG2	2.52	0.40
1:F:367:LYS:HB2	1:F:391:TYR:HE1	1.86	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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



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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	415/444 (94%)	359 (86%)	41 (10%)	15 (4%)	3	29
1	B	415/444 (94%)	357 (86%)	47 (11%)	11 (3%)	5	34
1	C	415/444 (94%)	365 (88%)	38 (9%)	12 (3%)	4	33
1	D	403/444 (91%)	355 (88%)	40 (10%)	8 (2%)	7	40
1	E	415/444 (94%)	358 (86%)	43 (10%)	14 (3%)	3	30
1	F	415/444 (94%)	354 (85%)	46 (11%)	15 (4%)	3	29
All	All	2478/2664 (93%)	2148 (87%)	255 (10%)	75 (3%)	4	32

All (75) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	44	LYS
1	A	157	ILE
1	A	255	LYS
1	A	258	ARG
1	A	316	TYR
1	A	375	ARG
1	B	44	LYS
1	B	166	GLU
1	B	255	LYS
1	B	258	ARG
1	B	316	TYR
1	B	375	ARG
1	C	44	LYS
1	C	175	ILE
1	C	255	LYS
1	C	258	ARG
1	C	316	TYR
1	C	375	ARG
1	D	44	LYS
1	D	255	LYS
1	D	258	ARG
1	D	316	TYR
1	D	375	ARG
1	E	165	TYR
1	E	168	ILE
1	E	170	SER
1	E	255	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	E	258	ARG
1	E	316	TYR
1	E	375	ARG
1	F	151	ASP
1	F	175	ILE
1	F	255	LYS
1	F	258	ARG
1	F	316	TYR
1	F	375	ARG
1	B	157	ILE
1	B	193	LYS
1	C	173	GLY
1	C	193	LYS
1	D	193	LYS
1	E	44	LYS
1	E	159	GLU
1	E	166	GLU
1	E	172	ASP
1	E	193	LYS
1	F	44	LYS
1	F	154	ASP
1	F	173	GLY
1	A	70	ARG
1	A	94	THR
1	A	172	ASP
1	A	193	LYS
1	B	158	ASP
1	F	193	LYS
1	A	27	PRO
1	F	379	GLN
1	A	147	ALA
1	A	149	GLY
1	A	254	ILE
1	B	27	PRO
1	C	170	SER
1	C	379	GLN
1	D	379	GLN
1	F	153	ASP
1	F	159	GLU
1	A	379	GLN
1	B	153	ASP
1	C	27	PRO

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Mol	Chain	Res	Type
1	E	379	GLN
1	F	254	ILE
1	C	124	VAL
1	F	157	ILE
1	D	27	PRO
1	E	27	PRO

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	361/386 (94%)	348 (96%)	13 (4%)	35 61
1	B	361/386 (94%)	343 (95%)	18 (5%)	24 53
1	C	361/386 (94%)	350 (97%)	11 (3%)	41 64
1	D	354/386 (92%)	345 (98%)	9 (2%)	47 69
1	E	361/386 (94%)	346 (96%)	15 (4%)	30 57
1	F	361/386 (94%)	347 (96%)	14 (4%)	32 59
All	All	2159/2316 (93%)	2079 (96%)	80 (4%)	34 60

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ILE
1	A	64	PHE
1	A	71	VAL
1	A	152	ASP
1	A	157	ILE
1	A	158	ASP
1	A	174	ASN
1	A	231	LEU
1	A	254	ILE
1	A	308	LYS
1	A	316	TYR
1	A	376	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	380	LEU
1	B	30	ILE
1	B	64	PHE
1	B	101	CYS
1	B	144	GLU
1	B	157	ILE
1	B	161	LEU
1	B	165	TYR
1	B	166	GLU
1	B	174	ASN
1	B	231	LEU
1	B	254	ILE
1	B	308	LYS
1	B	316	TYR
1	B	319	LEU
1	B	348	ASP
1	B	368	ARG
1	B	376	GLU
1	B	380	LEU
1	C	30	ILE
1	C	64	PHE
1	C	144	GLU
1	C	166	GLU
1	C	174	ASN
1	C	231	LEU
1	C	254	ILE
1	C	308	LYS
1	C	316	TYR
1	C	376	GLU
1	C	380	LEU
1	D	30	ILE
1	D	64	PHE
1	D	165	TYR
1	D	167	GLU
1	D	231	LEU
1	D	308	LYS
1	D	316	TYR
1	D	376	GLU
1	D	380	LEU
1	E	30	ILE
1	E	64	PHE
1	E	144	GLU

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Mol	Chain	Res	Type
1	E	153	ASP
1	E	159	GLU
1	E	165	TYR
1	E	167	GLU
1	E	174	ASN
1	E	231	LEU
1	E	308	LYS
1	E	316	TYR
1	E	319	LEU
1	E	368	ARG
1	E	376	GLU
1	E	380	LEU
1	F	30	ILE
1	F	64	PHE
1	F	125	ASN
1	F	150	THR
1	F	157	ILE
1	F	174	ASN
1	F	198	VAL
1	F	231	LEU
1	F	308	LYS
1	F	316	TYR
1	F	319	LEU
1	F	348	ASP
1	F	376	GLU
1	F	380	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (118) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	HIS
1	A	45	HIS
1	A	77	GLN
1	A	100	HIS
1	A	102	GLN
1	A	109	GLN
1	A	119	GLN
1	A	123	ASN
1	A	196	ASN
1	A	215	GLN
1	A	229	HIS
1	A	280	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	282	ASN
1	A	292	ASN
1	A	305	ASN
1	A	326	ASN
1	A	331	ASN
1	A	356	GLN
1	A	365	GLN
1	A	404	ASN
1	B	39	HIS
1	B	45	HIS
1	B	77	GLN
1	B	99	GLN
1	B	102	GLN
1	B	109	GLN
1	B	119	GLN
1	B	123	ASN
1	B	125	ASN
1	B	196	ASN
1	B	215	GLN
1	B	229	HIS
1	B	280	ASN
1	B	282	ASN
1	B	305	ASN
1	B	326	ASN
1	B	331	ASN
1	B	365	GLN
1	B	382	GLN
1	B	404	ASN
1	C	39	HIS
1	C	77	GLN
1	C	100	HIS
1	C	102	GLN
1	C	109	GLN
1	C	119	GLN
1	C	123	ASN
1	C	174	ASN
1	C	196	ASN
1	C	215	GLN
1	C	222	ASN
1	C	229	HIS
1	C	280	ASN
1	C	282	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	305	ASN
1	C	326	ASN
1	C	331	ASN
1	C	356	GLN
1	C	365	GLN
1	C	404	ASN
1	D	39	HIS
1	D	45	HIS
1	D	77	GLN
1	D	99	GLN
1	D	102	GLN
1	D	109	GLN
1	D	119	GLN
1	D	123	ASN
1	D	196	ASN
1	D	215	GLN
1	D	222	ASN
1	D	229	HIS
1	D	280	ASN
1	D	282	ASN
1	D	305	ASN
1	D	326	ASN
1	D	331	ASN
1	D	365	GLN
1	D	379	GLN
1	D	404	ASN
1	E	39	HIS
1	E	77	GLN
1	E	100	HIS
1	E	102	GLN
1	E	109	GLN
1	E	119	GLN
1	E	123	ASN
1	E	196	ASN
1	E	215	GLN
1	E	222	ASN
1	E	229	HIS
1	E	252	GLN
1	E	280	ASN
1	E	282	ASN
1	E	305	ASN
1	E	326	ASN

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Mol	Chain	Res	Type
1	E	331	ASN
1	E	365	GLN
1	E	404	ASN
1	F	39	HIS
1	F	77	GLN
1	F	99	GLN
1	F	102	GLN
1	F	109	GLN
1	F	119	GLN
1	F	123	ASN
1	F	196	ASN
1	F	215	GLN
1	F	222	ASN
1	F	229	HIS
1	F	280	ASN
1	F	282	ASN
1	F	300	GLN
1	F	305	ASN
1	F	326	ASN
1	F	331	ASN
1	F	365	GLN
1	F	404	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

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	419/444 (94%)	0.58	28 (6%) 17 14	103, 118, 142, 151	0
1	B	419/444 (94%)	0.64	35 (8%) 11 10	103, 117, 142, 151	0
1	C	419/444 (94%)	1.41	120 (28%) 0 0	103, 117, 142, 151	0
1	D	409/444 (92%)	1.40	98 (23%) 0 0	103, 117, 142, 151	0
1	E	419/444 (94%)	1.41	113 (26%) 0 0	103, 117, 142, 151	0
1	F	419/444 (94%)	0.95	64 (15%) 2 2	103, 117, 142, 151	0
All	All	2504/2664 (93%)	1.06	458 (18%) 1 1	103, 117, 142, 151	0

All (458) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	263	SER	10.0
1	C	365	GLN	9.2
1	D	434	ASN	8.9
1	A	256	ALA	8.6
1	D	435	LEU	7.7
1	F	365	GLN	7.7
1	C	402	SER	7.6
1	C	271	MET	7.2
1	E	79	GLY	6.9
1	C	358	SER	6.8
1	B	399	GLU	6.4
1	F	363	GLN	6.2
1	B	152	ASP	6.0
1	A	255	LYS	5.9
1	F	159	GLU	5.8
1	D	262	ALA	5.7
1	E	174	ASN	5.7
1	E	376	GLU	5.6
1	E	32	GLU	5.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	158	ASP	5.5
1	A	260	ASP	5.4
1	C	260	ASP	5.4
1	C	272	ALA	5.4
1	C	397	ASP	5.3
1	D	260	ASP	5.3
1	C	400	SER	5.2
1	D	32	GLU	5.2
1	D	250	ASN	5.2
1	E	77	GLN	5.1
1	E	171	ALA	5.1
1	F	364	ARG	5.0
1	C	279	SER	5.0
1	D	366	ASP	5.0
1	D	308	LYS	4.9
1	E	134	PRO	4.9
1	F	252	GLN	4.9
1	E	280	ASN	4.8
1	E	61	SER	4.6
1	E	375	ARG	4.6
1	E	401	GLU	4.6
1	E	377	SER	4.5
1	C	58	LYS	4.5
1	F	12	ASN	4.4
1	E	78	LEU	4.4
1	D	306	PRO	4.4
1	C	141	GLU	4.4
1	F	90	SER	4.4
1	C	267	GLY	4.4
1	E	119	GLN	4.4
1	E	223	ASP	4.3
1	F	260	ASP	4.3
1	D	399	GLU	4.3
1	D	179	PRO	4.3
1	E	260	ASP	4.2
1	E	158	ASP	4.2
1	C	398	LYS	4.2
1	E	100	HIS	4.2
1	E	72	GLY	4.1
1	D	113	ALA	4.1
1	F	434	ASN	4.1
1	E	172	ASP	4.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	259	ARG	4.1
1	C	326	ASN	4.1
1	E	250	ASN	4.1
1	D	157	ILE	4.1
1	F	170	SER	4.0
1	D	252	GLN	4.0
1	E	251	ALA	4.0
1	E	252	GLN	4.0
1	F	415	ASP	4.0
1	E	133	LYS	4.0
1	C	134	PRO	4.0
1	E	166	GLU	3.9
1	D	417	PRO	3.9
1	F	398	LYS	3.9
1	C	367	LYS	3.9
1	B	306	PRO	3.9
1	E	62	VAL	3.8
1	C	403	LYS	3.8
1	C	307	GLY	3.8
1	D	303	ARG	3.8
1	C	57	ARG	3.8
1	E	141	GLU	3.8
1	B	304	LYS	3.8
1	D	307	GLY	3.8
1	F	358	SER	3.8
1	C	32	GLU	3.8
1	F	366	ASP	3.8
1	C	360	GLN	3.7
1	E	75	LEU	3.7
1	E	303	ARG	3.7
1	E	123	ASN	3.7
1	D	190	TYR	3.7
1	E	33	CYS	3.7
1	C	427	LYS	3.7
1	D	436	GLU	3.7
1	E	326	ASN	3.7
1	E	27	PRO	3.7
1	C	359	ARG	3.6
1	C	224	ASP	3.6
1	F	91	VAL	3.6
1	D	180	SER	3.6
1	D	404	ASN	3.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	114	ILE	3.6
1	A	151	ASP	3.5
1	A	257	ALA	3.5
1	B	398	LYS	3.5
1	E	157	ILE	3.5
1	D	402	SER	3.5
1	E	436	GLU	3.5
1	E	256	ALA	3.5
1	D	159	GLU	3.5
1	E	151	ASP	3.5
1	C	372	SER	3.5
1	E	73	GLU	3.5
1	C	406	VAL	3.4
1	D	405	ILE	3.4
1	D	61	SER	3.4
1	E	304	LYS	3.4
1	B	153	ASP	3.4
1	C	323	ALA	3.4
1	C	29	LEU	3.4
1	C	145	ILE	3.4
1	C	391	TYR	3.4
1	C	324	LYS	3.4
1	F	436	GLU	3.4
1	E	125	ASN	3.3
1	C	366	ASP	3.3
1	F	140	SER	3.3
1	E	136	GLN	3.3
1	C	289	GLN	3.3
1	D	209	THR	3.3
1	E	246	ALA	3.3
1	A	141	GLU	3.3
1	C	305	ASN	3.3
1	B	132	VAL	3.3
1	E	282	ASN	3.3
1	F	258	ARG	3.3
1	E	179	PRO	3.2
1	E	173	GLY	3.2
1	A	174	ASN	3.2
1	F	402	SER	3.2
1	E	235	LYS	3.2
1	D	305	ASN	3.2
1	F	154	ASP	3.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	F	397	ASP	3.2
1	D	258	ARG	3.2
1	E	272	ALA	3.2
1	C	308	LYS	3.2
1	E	14	TYR	3.2
1	E	247	GLY	3.2
1	F	327	ASP	3.1
1	E	163	THR	3.1
1	A	123	ASN	3.1
1	E	302	LYS	3.1
1	E	273	ILE	3.1
1	E	162	VAL	3.1
1	F	263	SER	3.1
1	C	144	GLU	3.1
1	E	137	GLU	3.1
1	D	323	ALA	3.1
1	D	401	GLU	3.1
1	E	347	LEU	3.1
1	E	233	MET	3.0
1	A	376	GLU	3.0
1	C	303	ARG	3.0
1	D	368	ARG	3.0
1	C	304	LYS	3.0
1	D	422	SER	3.0
1	E	80	GLY	3.0
1	E	140	SER	3.0
1	D	29	LEU	3.0
1	C	399	GLU	3.0
1	C	325	ALA	3.0
1	C	209	THR	3.0
1	C	310	VAL	3.0
1	E	348	ASP	3.0
1	B	225	VAL	3.0
1	B	327	ASP	3.0
1	F	172	ASP	3.0
1	D	365	GLN	3.0
1	F	248	SER	3.0
1	E	227	ASN	3.0
1	D	169	GLU	2.9
1	F	78	LEU	2.9
1	D	253	LYS	2.9
1	D	227	ASN	2.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	151	ASP	2.9
1	D	134	PRO	2.9
1	A	159	GLU	2.9
1	B	305	ASN	2.9
1	E	310	VAL	2.9
1	F	158	ASP	2.9
1	D	183	THR	2.9
1	C	348	ASP	2.9
1	B	141	GLU	2.9
1	D	222	ASN	2.9
1	E	122	GLU	2.9
1	F	264	GLU	2.9
1	D	176	THR	2.8
1	D	299	ARG	2.8
1	F	401	GLU	2.8
1	C	368	ARG	2.8
1	D	48	ILE	2.8
1	D	304	LYS	2.8
1	F	307	GLY	2.8
1	B	415	ASP	2.8
1	E	169	GLU	2.8
1	F	324	LYS	2.8
1	E	245	THR	2.8
1	C	190	TYR	2.8
1	F	359	ARG	2.8
1	C	306	PRO	2.8
1	D	322	PRO	2.8
1	C	349	VAL	2.8
1	C	53	GLN	2.8
1	C	94	THR	2.8
1	F	435	LEU	2.8
1	E	152	ASP	2.8
1	C	261	PHE	2.8
1	C	436	GLU	2.8
1	C	223	ASP	2.8
1	E	258	ARG	2.7
1	E	419	GLY	2.7
1	C	292	ASN	2.7
1	C	270	SER	2.7
1	E	30	ILE	2.7
1	C	250	ASN	2.7
1	D	27	PRO	2.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	E	281	ILE	2.7
1	A	263	SER	2.7
1	D	414	ARG	2.7
1	D	60	GLN	2.7
1	D	109	GLN	2.7
1	A	172	ASP	2.7
1	D	247	GLY	2.7
1	C	27	PRO	2.7
1	C	34	PRO	2.7
1	D	406	VAL	2.7
1	E	175	ILE	2.7
1	F	422	SER	2.7
1	B	326	ASN	2.7
1	C	205	SER	2.7
1	B	144	GLU	2.7
1	C	435	LEU	2.7
1	D	26	GLU	2.7
1	E	184	GLU	2.7
1	C	269	LEU	2.7
1	C	315	ASP	2.7
1	F	253	LYS	2.7
1	C	158	ASP	2.7
1	C	136	GLN	2.7
1	C	79	GLY	2.7
1	C	125	ASN	2.7
1	D	140	SER	2.6
1	D	144	GLU	2.6
1	E	269	LEU	2.6
1	E	58	LYS	2.6
1	E	431	ASN	2.6
1	B	375	ARG	2.6
1	E	156	SER	2.6
1	F	183	THR	2.6
1	E	12	ASN	2.6
1	F	400	SER	2.6
1	E	257	ALA	2.6
1	A	365	GLN	2.6
1	E	170	SER	2.6
1	B	376	GLU	2.6
1	C	77	GLN	2.6
1	A	62	VAL	2.6
1	D	62	VAL	2.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	E	76	PRO	2.6
1	C	273	ILE	2.6
1	C	193	LYS	2.6
1	D	255	LYS	2.6
1	C	285	ASP	2.6
1	C	364	ARG	2.6
1	C	422	SER	2.6
1	D	264	GLU	2.5
1	E	404	ASN	2.5
1	F	92	ALA	2.5
1	C	122	GLU	2.5
1	B	223	ASP	2.5
1	E	434	ASN	2.5
1	C	392	ARG	2.5
1	D	72	GLY	2.5
1	A	348	ASP	2.5
1	D	392	ARG	2.5
1	D	118	GLN	2.5
1	E	15	ALA	2.5
1	F	136	GLN	2.5
1	C	275	GLU	2.5
1	E	301	THR	2.5
1	F	169	GLU	2.5
1	C	251	ALA	2.5
1	B	365	GLN	2.5
1	F	261	PHE	2.5
1	F	45	HIS	2.5
1	C	394	ASP	2.5
1	C	208	LYS	2.5
1	A	304	LYS	2.5
1	C	238	ASN	2.5
1	D	398	LYS	2.5
1	F	433	VAL	2.5
1	D	327	ASP	2.4
1	D	175	ILE	2.4
1	E	241	ARG	2.4
1	E	279	SER	2.4
1	D	400	SER	2.4
1	F	94	THR	2.4
1	F	393	ASP	2.4
1	C	282	ASN	2.4
1	C	309	ARG	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	265	ASP	2.4
1	E	222	ASN	2.4
1	D	364	ARG	2.4
1	A	170	SER	2.4
1	C	405	ILE	2.4
1	F	399	GLU	2.4
1	A	303	ARG	2.4
1	E	194	ARG	2.4
1	A	254	ILE	2.4
1	E	234	GLY	2.4
1	E	255	LYS	2.4
1	F	29	LEU	2.4
1	C	56	ASP	2.4
1	F	62	VAL	2.4
1	E	74	LYS	2.4
1	E	110	LYS	2.4
1	D	375	ARG	2.4
1	D	132	VAL	2.4
1	E	22	SER	2.4
1	B	121	ILE	2.3
1	C	301	THR	2.4
1	B	266	TRP	2.3
1	A	326	ASN	2.3
1	D	309	ARG	2.3
1	E	399	GLU	2.3
1	E	262	ALA	2.3
1	F	150	THR	2.3
1	E	168	ILE	2.3
1	B	101	CYS	2.3
1	F	171	ALA	2.3
1	A	265	ASP	2.3
1	F	153	ASP	2.3
1	C	276	ILE	2.3
1	E	116	ILE	2.3
1	A	307	GLY	2.3
1	C	74	LYS	2.3
1	B	363	GLN	2.3
1	C	227	ASN	2.3
1	A	122	GLU	2.3
1	D	193	LYS	2.3
1	E	428	GLU	2.3
1	C	281	ILE	2.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	E	244	VAL	2.3
1	C	278	ASN	2.3
1	C	429	TYR	2.3
1	D	18	ALA	2.3
1	D	413	HIS	2.3
1	F	20	LEU	2.3
1	C	343	MET	2.2
1	D	230	SER	2.2
1	C	262	ALA	2.2
1	F	262	ALA	2.2
1	B	90	SER	2.2
1	D	415	ASP	2.2
1	B	377	SER	2.2
1	A	136	GLN	2.2
1	C	420	THR	2.2
1	E	63	ASP	2.2
1	C	255	LYS	2.2
1	C	345	ARG	2.2
1	E	31	LYS	2.2
1	F	165	TYR	2.2
1	B	72	GLY	2.2
1	C	246	ALA	2.2
1	C	342	LYS	2.2
1	B	260	ASP	2.2
1	F	377	SER	2.2
1	D	290	SER	2.2
1	F	141	GLU	2.2
1	D	160	ALA	2.2
1	D	232	GLU	2.2
1	D	22	SER	2.2
1	E	92	ALA	2.2
1	C	135	ILE	2.2
1	D	287	ALA	2.2
1	C	12	ASN	2.2
1	C	256	ALA	2.2
1	D	256	ALA	2.2
1	D	357	LEU	2.2
1	F	161	LEU	2.2
1	C	300	GLN	2.2
1	D	145	ILE	2.2
1	E	60	GLN	2.2
1	A	358	SER	2.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	196	ASN	2.1
1	B	118	GLN	2.1
1	C	254	ILE	2.1
1	C	295	TRP	2.1
1	C	424	ALA	2.1
1	C	414	ARG	2.1
1	E	167	GLU	2.1
1	F	117	ALA	2.1
1	C	140	SER	2.1
1	D	59	GLY	2.1
1	E	331	ASN	2.1
1	E	379	GLN	2.1
1	D	300	GLN	2.1
1	B	434	ASN	2.1
1	F	396	TYR	2.1
1	C	219	MET	2.1
1	C	415	ASP	2.1
1	B	431	ASN	2.1
1	C	327	ASP	2.1
1	D	96	THR	2.1
1	E	190	TYR	2.1
1	F	270	SER	2.1
1	E	274	GLY	2.1
1	C	291	VAL	2.1
1	D	217	LYS	2.1
1	E	118	GLN	2.1
1	C	159	GLU	2.1
1	C	385	ASP	2.1
1	E	265	ASP	2.1
1	F	106	GLU	2.1
1	D	433	VAL	2.1
1	D	266	TRP	2.1
1	D	331	ASN	2.1
1	D	182	PHE	2.1
1	F	110	LYS	2.1
1	A	235	LYS	2.0
1	E	261	PHE	2.1
1	F	367	LYS	2.0
1	C	54	ASP	2.0
1	D	416	GLY	2.0
1	E	324	LYS	2.0
1	C	176	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	194	ARG	2.0
1	C	268	LYS	2.0
1	C	62	VAL	2.0
1	D	403	LYS	2.0
1	F	326	ASN	2.0
1	B	224	ASP	2.0
1	C	28	GLU	2.0
1	E	224	ASP	2.0
1	A	259	ARG	2.0
1	B	292	ASN	2.0
1	D	257	ALA	2.0
1	D	259	ARG	2.0
1	B	255	LYS	2.0
1	B	25	THR	2.0
1	D	397	ASP	2.0
1	D	133	LYS	2.0
1	A	258	ARG	2.0
1	E	135	ILE	2.0
1	B	307	GLY	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.