



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 11:26 PM GMT

PDB ID : 3A5D
Title : Inter-subunit interaction and quaternary rearrangement defined by the central stalk of prokaryotic V1-ATPase
Authors : Numoto, N.; Hasegawa, Y.; Takeda, K.; Miki, K.
Deposited on : 2009-08-06
Resolution : 4.80 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

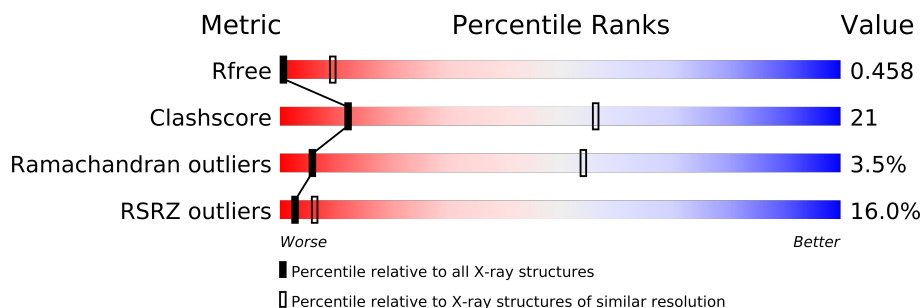
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 4.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1046 (6.00-3.50)
Clashscore	79885	1320 (6.00-3.50)
Ramachandran outliers	78287	1236 (6.00-3.50)
RSRZ outliers	66119	1045 (6.00-3.50)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	578	
1	B	578	
1	C	578	
1	I	578	
1	J	578	
1	K	578	
2	D	478	
2	E	478	
2	F	478	
2	L	478	
2	M	478	
2	N	478	
3	G	223	
3	O	223	
4	H	104	
4	P	104	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 32080 atoms, of which 0 are hydrogen and 0 are deuterium.

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 V-type ATP synthase alpha chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	561	Total	C	N	O	0	0	0
			2752	1630	561	561			
1	B	561	Total	C	N	O	0	0	0
			2752	1630	561	561			
1	C	561	Total	C	N	O	0	0	0
			2752	1630	561	561			
1	I	561	Total	C	N	O	0	0	0
			2752	1630	561	561			
1	J	561	Total	C	N	O	0	0	0
			2752	1630	561	561			
1	K	561	Total	C	N	O	0	0	0
			2752	1630	561	561			

- Molecule 2 is a protein called V-type ATP synthase beta chain.

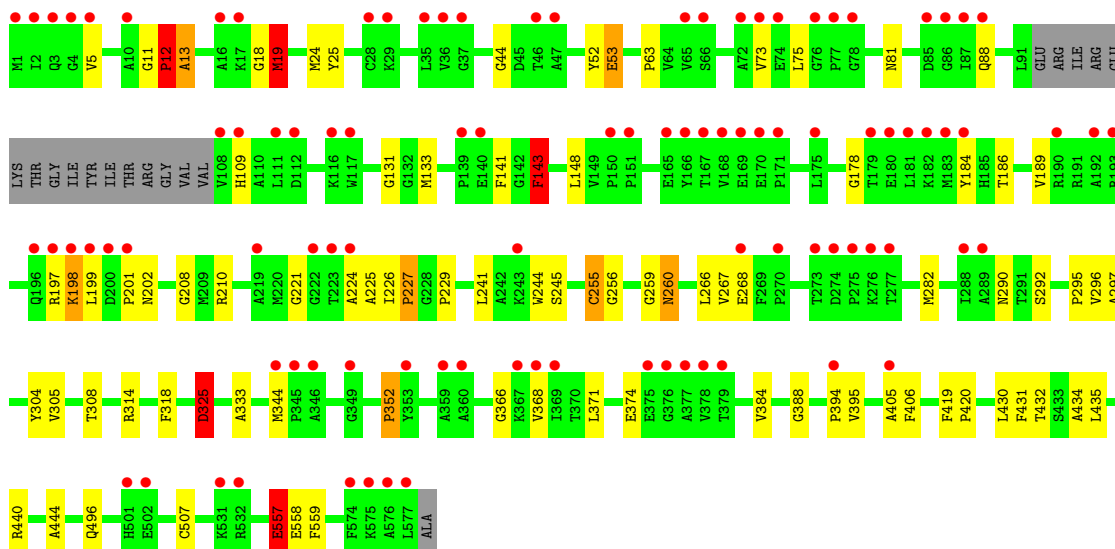
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	450	Total	C	N	O	0	0	0
			2212	1312	450	450			
2	E	450	Total	C	N	O	0	0	0
			2212	1312	450	450			
2	F	450	Total	C	N	O	0	0	0
			2212	1312	450	450			
2	L	450	Total	C	N	O	0	0	0
			2212	1312	450	450			
2	M	450	Total	C	N	O	0	0	0
			2212	1312	450	450			
2	N	450	Total	C	N	O	0	0	0
			2212	1312	450	450			

- Molecule 3 is a protein called V-type ATP synthase subunit D.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	129	Total 639	C 381	N 129	O 129	0	0	0
3	O	129	Total 639	C 381	N 129	O 129	0	0	0

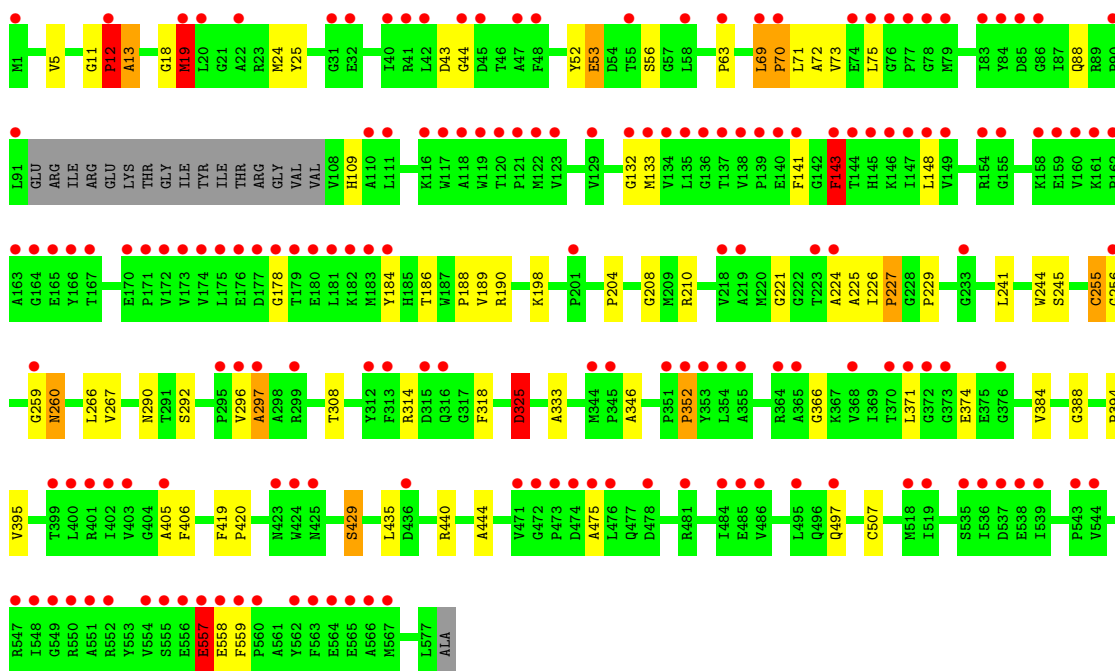
- Molecule 4 is a protein called V-type ATP synthase subunit F.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	H	104	Total 509	C 301	N 104	O 104	0	0	0
4	P	104	Total 509	C 301	N 104	O 104	0	0	0



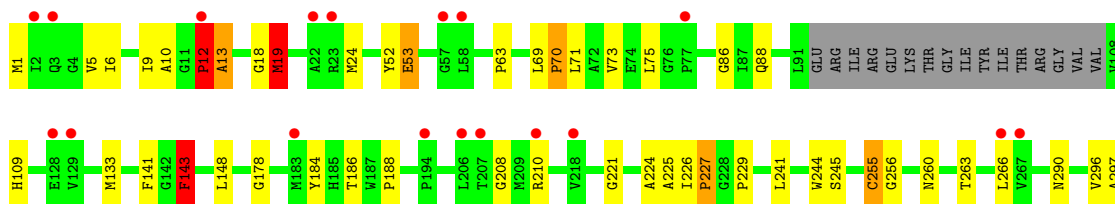
• Molecule 1: V-type ATP synthase alpha chain

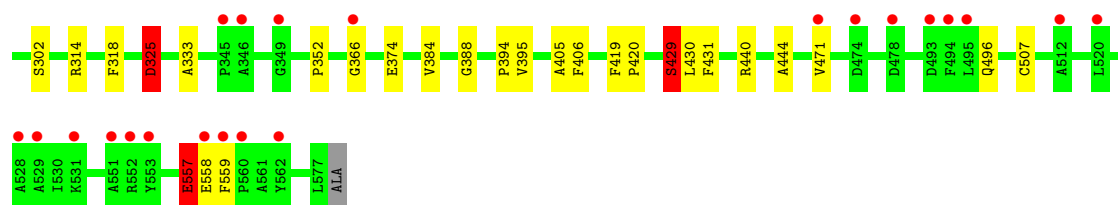
Chain I:



• Molecule 1: V-type ATP synthase alpha chain

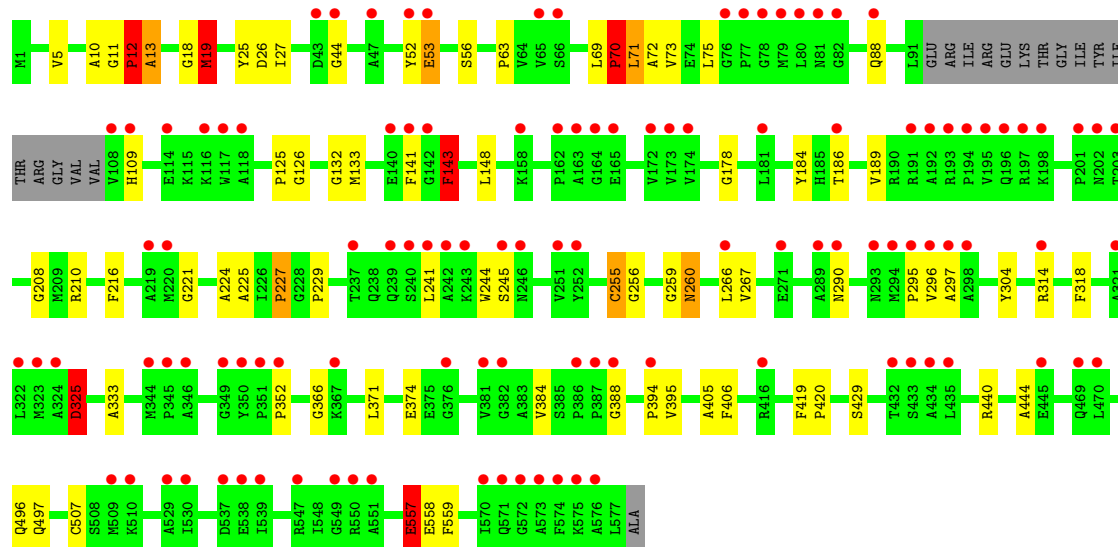
Chain J:





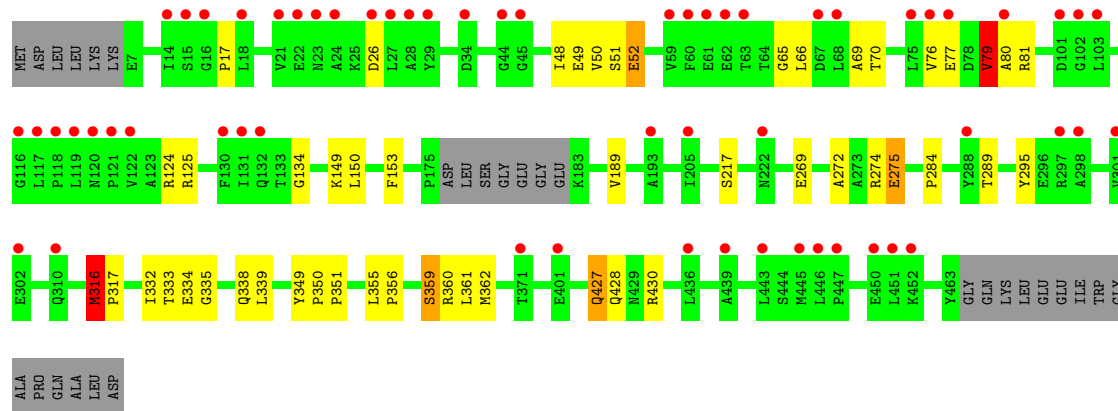
• Molecule 1: V-type ATP synthase alpha chain

Chain K:



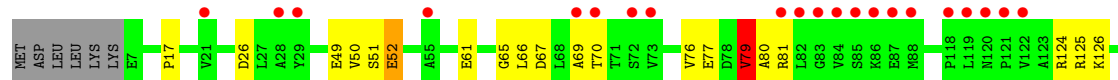
• Molecule 2: V-type ATP synthase beta chain

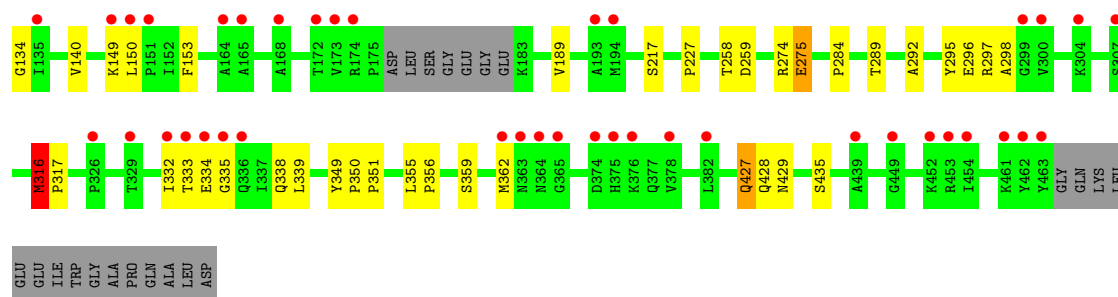
Chain D:



• Molecule 2: V-type ATP synthase beta chain

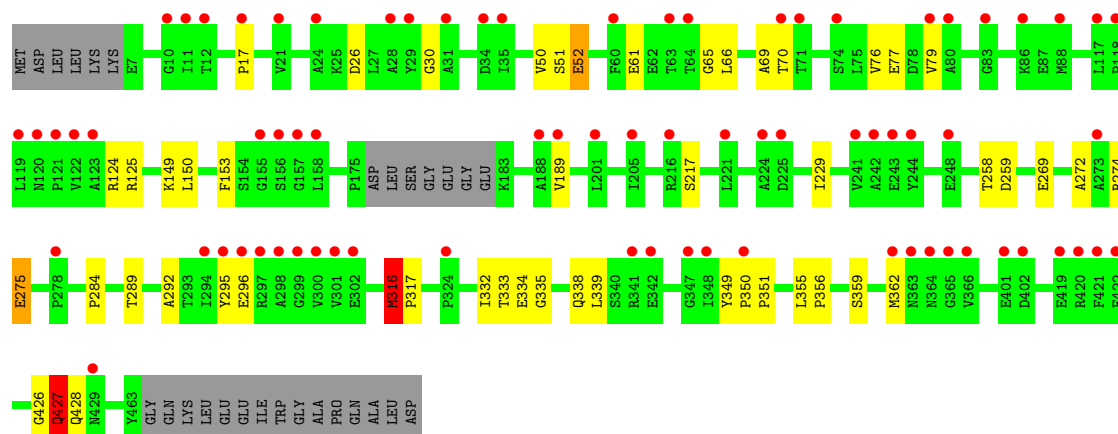
Chain E:





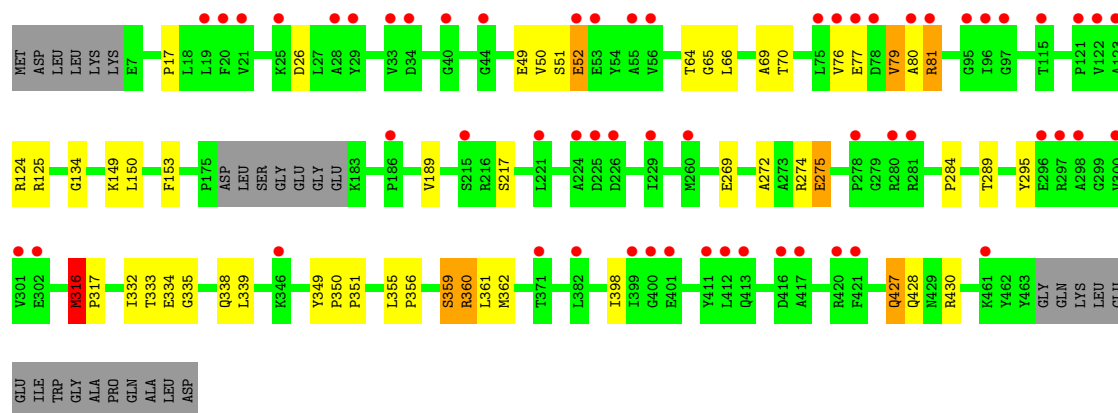
• Molecule 2: V-type ATP synthase beta chain

Chain F:



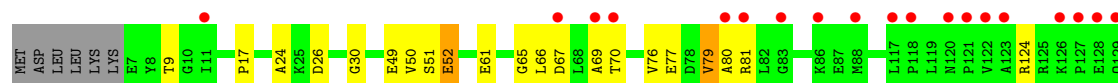
• Molecule 2: V-type ATP synthase beta chain

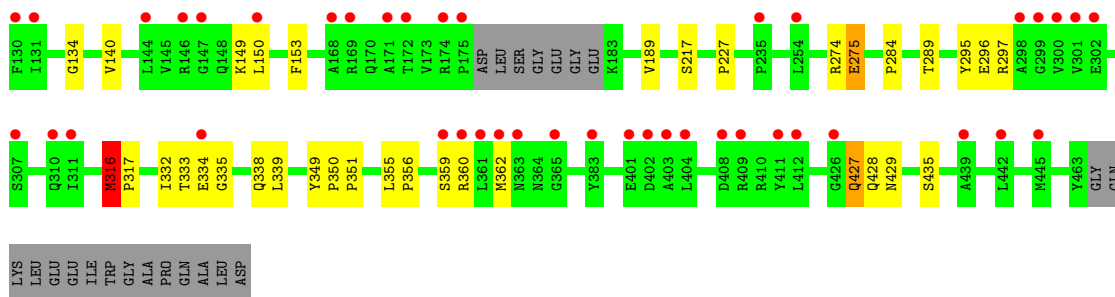
Chain L:



• Molecule 2: V-type ATP synthase beta chain

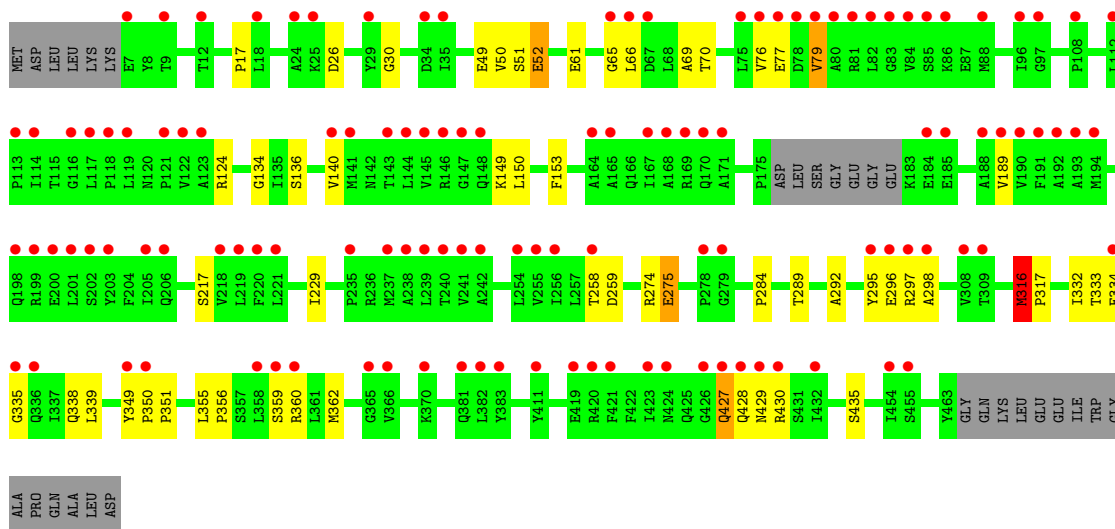
Chain M:





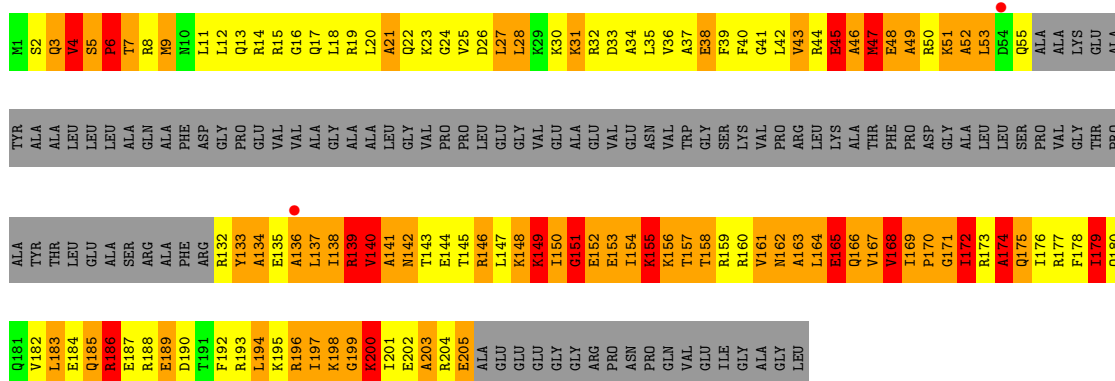
- Molecule 2: V-type ATP synthase beta chain

Chain N:



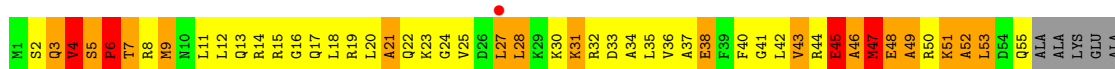
- Molecule 3: V-type ATP synthase subunit D

Chain G:



- Molecule 3: V-type ATP synthase subunit D

Chain 0:



TYR
ALA
ALA
LEU
LEU
LEU
ALA
GLN
ALA
PHE
ASP
GLY
PRO
GLU
VAL
VAL
ALA
GLY
ALA
ALA
LEU
GLY
VAL
PRO
PRO
LEU
GLU
GLY
VAL
GLU
ALA
GLU
VAL
GLU
ASN
VAL
TRP
GLY
SER
LYS
VAL
PRO
PRO
ARG
LEU
LYS
ALA
THR
PHE
PRO
ASP
GLY
ALA
LEU
SER
PRO
VAL
GLY
THR
PRO

ALA
TYR
THR
GLU
GLU
ALA
SER
ARG
PHE
D190
ARG
R132
Y133
A134
E135
A136
I137
I138
I139
Y140
A141
N142
T143
E144
T145
R146
L147
K148
K149
I150
G151
E152
E153
I154
K155
K156
T157
T158
R159
R160
V161
N162
A163
L164
E165
Q166
V167
V168
I169
P170
G171
I172
R173
A174
Q175
I176
R177
F178
I179
Q180

Q181
V182
L183
E184
Q185
R186
S24
E187
R188
E189
D190
T191
F192
R193
L194
K195
R196
I197
K198
G199
K200
I201
E202
A203
R204
E205
ALA
GLU
GLU
GLU
GLY
GLY
ARG
PRO
ASN
PRO
GLN
VAL
GLU
ILE
GLY
ALA
GLY
LEU

● Molecule 4: V-type ATP synthase subunit F

Chain H:

W1
A16
A23
S25
A29
E34
E38
G40
L62
M63
R64
G65
R66
I74
A75
G76
L77
K78
E79
A80
F81
Q82
G83
H84
D85
V86
I98
G99
F100
D101
I102
K103
L104

● Molecule 4: V-type ATP synthase subunit F

Chain P:

W1
A16
S25
A29
E34
T35
R39
G40
L62
M63
R64
G65
R66
I74
A75
G76
L77
K78
Q82
G83
H84
D85
V86
E87
G88
Y89
V94
R95
I98
G99
F100
L104

4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	380.70Å 380.70Å 147.97Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.97 – 4.80 49.72 – 4.80	Depositor EDS
% Data completeness (in resolution range)	95.3 (29.97-4.80) 95.2 (49.72-4.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 4.86Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.441 , 0.454 0.446 , 0.458	Depositor DCC
R_{free} test set	2935 reflections (5.42%)	DCC
Wilson B-factor (Å ²)	173.9	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	-0.00 , -10.0	EDS
Estimated twinning fraction	0.217 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.28$, $\langle L^2 \rangle = 0.12$	Xtriage
Outliers	1 of 57297 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.69	EDS
Total number of atoms	32080	wwPDB-VP
Average B, all atoms (Å ²)	191.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.54% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.59	3/2750 (0.1%)	1.25	12/3815 (0.3%)
1	B	0.62	4/2750 (0.1%)	1.19	9/3815 (0.2%)
1	C	0.60	4/2750 (0.1%)	1.20	10/3815 (0.3%)
1	I	0.61	4/2750 (0.1%)	1.30	17/3815 (0.4%)
1	J	0.61	4/2750 (0.1%)	1.26	13/3815 (0.3%)
1	K	0.61	4/2750 (0.1%)	1.43	12/3815 (0.3%)
2	D	0.77	6/2210 (0.3%)	1.02	11/3068 (0.4%)
2	E	0.77	6/2210 (0.3%)	1.01	9/3068 (0.3%)
2	F	0.73	3/2210 (0.1%)	0.99	7/3068 (0.2%)
2	L	0.79	6/2210 (0.3%)	1.07	14/3068 (0.5%)
2	M	0.76	5/2210 (0.2%)	1.00	8/3068 (0.3%)
2	N	0.75	3/2210 (0.1%)	1.00	7/3068 (0.2%)
3	G	4.09	125/637 (19.6%)	2.63	49/885 (5.5%)
3	O	4.09	125/637 (19.6%)	2.63	50/885 (5.6%)
4	H	1.50	9/508 (1.8%)	1.43	10/703 (1.4%)
4	P	1.61	10/508 (2.0%)	2.13	17/703 (2.4%)
All	All	1.08	321/32050 (1.0%)	1.28	255/44474 (0.6%)

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	5
1	B	0	5
1	C	0	6
1	I	0	6
1	J	0	6
1	K	0	6
2	D	0	3
2	E	0	3
2	F	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	L	0	3
2	M	0	3
2	N	0	3
4	H	0	2
4	P	0	2
All	All	0	55

All (321) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	47	MET	CA-CB	-24.95	0.99	1.53
3	G	47	MET	CA-CB	-24.94	0.99	1.53
3	O	27	LEU	CA-CB	14.84	1.87	1.53
3	G	27	LEU	CA-CB	14.76	1.87	1.53
3	O	7	THR	CA-CB	12.80	1.86	1.53
3	G	7	THR	CA-CB	12.65	1.86	1.53
3	O	31	LYS	N-CA	12.38	1.71	1.46
3	G	31	LYS	N-CA	12.13	1.70	1.46
3	G	138	ILE	CA-CB	-12.12	1.26	1.54
3	G	196	ARG	CA-C	12.09	1.84	1.52
3	O	138	ILE	CA-CB	-12.07	1.27	1.54
3	O	196	ARG	CA-C	12.05	1.84	1.52
3	O	52	ALA	CA-CB	11.20	1.75	1.52
3	O	205	GLU	CA-CB	11.19	1.78	1.53
3	G	52	ALA	CA-CB	11.13	1.75	1.52
3	G	168	VAL	CA-CB	-11.09	1.31	1.54
3	G	16	GLY	CA-C	11.09	1.69	1.51
3	O	16	GLY	CA-C	11.07	1.69	1.51
3	G	205	GLU	CA-CB	10.99	1.78	1.53
3	O	168	VAL	CA-CB	-10.98	1.31	1.54
3	G	167	VAL	CA-C	10.89	1.81	1.52
3	O	167	VAL	CA-C	10.86	1.81	1.52
4	P	34	GLU	C-O	10.60	1.43	1.23
4	H	34	GLU	C-O	10.58	1.43	1.23
3	O	171	GLY	CA-C	10.55	1.68	1.51
3	G	171	GLY	CA-C	10.49	1.68	1.51
3	G	189	GLU	CA-CB	10.25	1.76	1.53
3	O	16	GLY	C-O	10.25	1.40	1.23
3	O	189	GLU	CA-CB	10.19	1.76	1.53
3	G	16	GLY	C-O	10.00	1.39	1.23
3	O	4	VAL	CA-C	9.78	1.78	1.52
3	G	4	VAL	CA-C	9.75	1.78	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	19	ARG	N-CA	9.49	1.65	1.46
3	G	19	ARG	N-CA	9.48	1.65	1.46
3	O	50	ARG	C-O	9.29	1.41	1.23
3	O	32	ARG	C-O	9.14	1.40	1.23
3	G	32	ARG	C-O	9.12	1.40	1.23
3	G	50	ARG	C-O	9.11	1.40	1.23
3	G	164	LEU	C-O	9.09	1.40	1.23
3	O	164	LEU	C-O	9.08	1.40	1.23
3	G	184	GLU	CA-CB	9.05	1.73	1.53
3	O	184	GLU	CA-CB	9.04	1.73	1.53
3	O	163	ALA	C-O	8.96	1.40	1.23
3	G	184	GLU	N-CA	8.95	1.64	1.46
3	G	6	PRO	C-O	8.94	1.41	1.23
3	O	184	GLU	N-CA	8.92	1.64	1.46
3	G	163	ALA	C-O	8.85	1.40	1.23
3	O	169	ILE	C-O	8.76	1.40	1.23
3	G	169	ILE	C-O	8.71	1.39	1.23
1	B	429	SER	C-N	8.70	1.54	1.34
3	O	6	PRO	C-O	8.68	1.40	1.23
3	O	142	ASN	CA-CB	8.66	1.75	1.53
3	G	183	LEU	C-O	8.60	1.39	1.23
3	G	142	ASN	CA-CB	8.60	1.75	1.53
3	G	194	LEU	CA-C	8.55	1.75	1.52
3	O	183	LEU	C-O	8.52	1.39	1.23
3	O	194	LEU	CA-C	8.46	1.75	1.52
3	G	163	ALA	CA-C	8.43	1.74	1.52
3	O	38	GLU	N-CA	8.40	1.63	1.46
3	O	163	ALA	CA-C	8.35	1.74	1.52
3	G	38	GLU	N-CA	8.32	1.62	1.46
3	G	182	VAL	N-CA	8.28	1.62	1.46
3	O	182	VAL	N-CA	8.27	1.62	1.46
4	P	40	GLY	C-O	8.20	1.36	1.23
4	H	40	GLY	C-O	8.10	1.36	1.23
4	P	75	ALA	N-CA	8.05	1.62	1.46
3	O	34	ALA	CA-CB	-8.04	1.35	1.52
3	G	34	ALA	CA-CB	-8.02	1.35	1.52
3	O	155	LYS	N-CA	8.01	1.62	1.46
3	G	155	LYS	N-CA	7.99	1.62	1.46
3	G	195	LYS	N-CA	7.96	1.62	1.46
3	O	205	GLU	CA-C	7.88	1.73	1.52
3	O	185	GLN	C-O	7.88	1.38	1.23
3	O	170	PRO	CA-C	7.87	1.68	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	195	LYS	N-CA	7.87	1.62	1.46
3	G	185	GLN	C-O	7.84	1.38	1.23
3	G	205	GLU	CA-C	7.82	1.73	1.52
3	G	170	PRO	CA-C	7.73	1.68	1.52
3	O	198	LYS	C-O	7.73	1.38	1.23
3	G	198	LYS	C-O	7.71	1.38	1.23
3	G	24	GLY	CA-C	7.67	1.64	1.51
3	G	46	ALA	C-O	7.62	1.37	1.23
3	G	192	PHE	C-O	7.56	1.37	1.23
3	O	46	ALA	C-O	7.56	1.37	1.23
3	O	24	GLY	CA-C	7.55	1.64	1.51
3	O	192	PHE	C-O	7.54	1.37	1.23
1	J	429	SER	C-N	7.47	1.51	1.34
3	O	51	LYS	C-O	7.46	1.37	1.23
3	G	134	ALA	CA-CB	7.46	1.68	1.52
3	O	4	VAL	CA-CB	7.44	1.70	1.54
3	G	4	VAL	CA-CB	7.42	1.70	1.54
1	K	70	PRO	C-N	7.42	1.51	1.34
3	G	33	ASP	N-CA	7.40	1.61	1.46
2	L	81	ARG	CA-C	7.40	1.72	1.52
3	O	33	ASP	N-CA	7.40	1.61	1.46
4	P	76	GLY	N-CA	7.37	1.57	1.46
3	G	51	LYS	C-O	7.37	1.37	1.23
3	O	134	ALA	CA-CB	7.37	1.68	1.52
3	O	134	ALA	N-CA	7.34	1.61	1.46
3	G	134	ALA	N-CA	7.32	1.60	1.46
3	G	167	VAL	CA-CB	7.31	1.70	1.54
3	O	146	ARG	CA-CB	7.31	1.70	1.53
4	P	75	ALA	CA-C	7.30	1.72	1.52
3	G	6	PRO	CA-CB	7.29	1.68	1.53
3	G	22	GLN	C-O	7.29	1.37	1.23
3	O	53	LEU	N-CA	7.28	1.60	1.46
3	G	146	ARG	CA-CB	7.26	1.70	1.53
2	L	81	ARG	N-CA	7.26	1.60	1.46
3	O	22	GLN	C-O	7.23	1.37	1.23
3	O	20	LEU	CA-C	7.22	1.71	1.52
3	G	20	LEU	CA-C	7.21	1.71	1.52
4	P	76	GLY	CA-C	7.20	1.63	1.51
3	O	167	VAL	CA-CB	7.18	1.69	1.54
3	O	6	PRO	CA-CB	7.16	1.67	1.53
3	G	193	ARG	N-CA	7.12	1.60	1.46
3	O	172	ILE	N-CA	7.11	1.60	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	172	ILE	N-CA	7.09	1.60	1.46
3	O	193	ARG	N-CA	7.09	1.60	1.46
3	O	27	LEU	N-CA	7.07	1.60	1.46
3	G	53	LEU	N-CA	7.07	1.60	1.46
3	G	188	ARG	N-CA	7.05	1.60	1.46
3	G	27	LEU	N-CA	7.05	1.60	1.46
3	G	154	ILE	C-O	7.05	1.36	1.23
3	O	188	ARG	N-CA	7.04	1.60	1.46
3	O	52	ALA	N-CA	6.99	1.60	1.46
2	L	80	ALA	CA-C	6.99	1.71	1.52
3	G	199	GLY	N-CA	6.96	1.56	1.46
3	G	179	ILE	C-O	6.96	1.36	1.23
4	P	77	LEU	N-CA	6.95	1.60	1.46
2	D	81	ARG	N-CA	6.95	1.60	1.46
3	G	4	VAL	C-O	6.95	1.36	1.23
3	G	52	ALA	N-CA	6.94	1.60	1.46
3	O	11	LEU	CA-CB	6.93	1.69	1.53
3	G	32	ARG	CA-C	6.92	1.71	1.52
3	G	156	LYS	CA-C	6.91	1.71	1.52
3	G	11	LEU	CA-CB	6.91	1.69	1.53
3	O	179	ILE	C-O	6.90	1.36	1.23
3	O	32	ARG	CA-C	6.89	1.70	1.52
3	O	156	LYS	CA-C	6.87	1.70	1.52
3	O	4	VAL	C-O	6.86	1.36	1.23
3	O	154	ILE	C-O	6.82	1.36	1.23
3	O	199	GLY	N-CA	6.71	1.56	1.46
2	E	81	ARG	N-CA	6.66	1.59	1.46
3	O	169	ILE	N-CA	6.63	1.59	1.46
3	G	204	ARG	N-CA	6.61	1.59	1.46
3	O	175	GLN	CA-CB	-6.60	1.39	1.53
3	G	5	SER	CA-CB	6.59	1.62	1.52
3	O	204	ARG	N-CA	6.57	1.59	1.46
3	G	17	GLN	CA-CB	-6.55	1.39	1.53
3	O	32	ARG	C-N	6.52	1.49	1.34
3	G	169	ILE	N-CA	6.51	1.59	1.46
3	G	189	GLU	CA-C	6.50	1.69	1.52
3	G	175	GLN	CA-CB	-6.48	1.39	1.53
3	O	148	LYS	CA-CB	6.48	1.68	1.53
3	O	17	GLN	CA-CB	-6.48	1.39	1.53
3	G	32	ARG	C-N	6.47	1.49	1.34
3	G	148	LYS	CA-CB	6.46	1.68	1.53
3	O	189	GLU	CA-C	6.44	1.69	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	14	ARG	N-CA	6.41	1.59	1.46
3	O	5	SER	CA-CB	6.39	1.62	1.52
3	O	9	MET	CA-C	-6.37	1.36	1.52
3	O	196	ARG	CA-CB	6.36	1.68	1.53
3	G	14	ARG	C-O	6.36	1.35	1.23
3	G	28	LEU	CA-C	6.35	1.69	1.52
3	O	31	LYS	C-O	6.33	1.35	1.23
3	G	196	ARG	CA-CB	6.32	1.67	1.53
3	G	9	MET	CA-C	-6.29	1.36	1.52
3	O	14	ARG	C-O	6.29	1.35	1.23
4	H	40	GLY	C-N	6.25	1.44	1.33
2	D	80	ALA	CA-C	6.21	1.69	1.52
3	O	14	ARG	N-CA	6.20	1.58	1.46
3	O	28	LEU	CA-C	6.19	1.69	1.52
3	O	192	PHE	CA-C	6.19	1.69	1.52
3	G	31	LYS	C-O	6.18	1.35	1.23
4	P	40	GLY	C-N	6.18	1.44	1.33
3	O	45	GLU	C-O	6.13	1.34	1.23
4	H	75	ALA	N-CA	6.13	1.58	1.46
3	O	24	GLY	C-O	6.13	1.33	1.23
3	G	192	PHE	CA-C	6.12	1.68	1.52
1	K	13	ALA	CA-CB	-6.09	1.39	1.52
1	J	13	ALA	CA-CB	-6.09	1.39	1.52
1	B	13	ALA	CA-CB	-6.08	1.39	1.52
3	G	164	LEU	N-CA	6.08	1.58	1.46
3	O	164	LEU	N-CA	6.06	1.58	1.46
3	O	194	LEU	C-O	6.05	1.34	1.23
3	O	201	ILE	CA-CB	-6.05	1.41	1.54
1	C	13	ALA	CA-CB	-6.05	1.39	1.52
1	A	13	ALA	CA-CB	-6.02	1.39	1.52
3	G	194	LEU	C-O	6.01	1.34	1.23
3	O	203	ALA	N-CA	-6.00	1.34	1.46
3	G	45	GLU	C-O	5.99	1.34	1.23
3	G	205	GLU	C-O	5.98	1.34	1.23
3	G	201	ILE	CA-CB	-5.98	1.41	1.54
3	O	205	GLU	C-O	5.98	1.34	1.23
1	I	13	ALA	CA-CB	-5.98	1.39	1.52
3	G	7	THR	CA-C	5.96	1.68	1.52
3	G	166	GLN	CA-CB	-5.96	1.40	1.53
3	O	7	THR	CA-C	5.95	1.68	1.52
2	E	80	ALA	CA-C	5.94	1.68	1.52
3	O	166	GLN	CA-CB	-5.92	1.41	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	24	GLY	C-O	5.85	1.33	1.23
3	G	203	ALA	N-CA	-5.83	1.34	1.46
3	G	21	ALA	C-O	5.81	1.34	1.23
3	G	37	ALA	CA-CB	-5.81	1.40	1.52
3	O	14	ARG	CA-CB	5.79	1.66	1.53
3	G	23	LYS	N-CA	5.73	1.57	1.46
3	O	141	ALA	CA-CB	5.73	1.64	1.52
2	M	81	ARG	N-CA	5.72	1.57	1.46
2	D	81	ARG	CA-C	5.72	1.67	1.52
3	O	23	LYS	N-CA	5.70	1.57	1.46
3	G	170	PRO	N-CA	5.69	1.56	1.47
3	O	21	ALA	C-O	5.69	1.34	1.23
3	O	52	ALA	C-O	5.69	1.34	1.23
2	N	275	GLU	CA-CB	-5.68	1.41	1.53
3	G	52	ALA	C-O	5.68	1.34	1.23
3	G	49	ALA	N-CA	5.67	1.57	1.46
3	O	37	ALA	CA-CB	-5.66	1.40	1.52
2	L	275	GLU	CA-CB	-5.64	1.41	1.53
2	M	275	GLU	CA-CB	-5.63	1.41	1.53
3	G	49	ALA	CA-CB	-5.62	1.40	1.52
4	H	25	SER	CA-CB	5.61	1.61	1.52
3	O	47	MET	C-O	5.60	1.33	1.23
2	E	275	GLU	CA-CB	-5.59	1.41	1.53
3	G	141	ALA	CA-CB	5.59	1.64	1.52
3	O	170	PRO	N-CA	5.58	1.56	1.47
3	G	14	ARG	CA-CB	5.58	1.66	1.53
3	O	171	GLY	C-O	5.58	1.32	1.23
3	G	158	THR	CA-CB	-5.57	1.38	1.53
3	G	25	VAL	N-CA	5.57	1.57	1.46
3	G	47	MET	C-O	5.57	1.33	1.23
2	F	275	GLU	CA-CB	-5.57	1.41	1.53
3	O	25	VAL	N-CA	5.57	1.57	1.46
3	G	148	LYS	N-CA	5.56	1.57	1.46
3	G	15	ARG	CA-CB	5.54	1.66	1.53
2	D	275	GLU	CA-CB	-5.54	1.41	1.53
2	L	289	THR	C-N	5.53	1.46	1.34
3	O	15	ARG	CA-CB	5.53	1.66	1.53
3	O	158	THR	CA-CB	-5.52	1.39	1.53
2	E	81	ARG	CA-C	5.52	1.67	1.52
3	O	49	ALA	N-CA	5.52	1.57	1.46
4	H	75	ALA	CA-C	5.51	1.67	1.52
3	O	148	LYS	N-CA	5.50	1.57	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	171	GLY	C-O	5.50	1.32	1.23
4	P	25	SER	CA-CB	5.49	1.61	1.52
3	O	187	GLU	CA-C	5.48	1.67	1.52
3	O	49	ALA	CA-CB	-5.45	1.41	1.52
3	G	36	VAL	CA-C	5.45	1.67	1.52
3	G	163	ALA	C-N	5.44	1.46	1.34
3	G	187	GLU	CA-C	5.44	1.67	1.52
3	O	163	ALA	C-N	5.43	1.46	1.34
3	O	7	THR	C-O	5.42	1.33	1.23
2	E	316	MET	C-N	-5.41	1.24	1.34
3	G	7	THR	C-O	5.40	1.33	1.23
2	L	316	MET	C-N	-5.39	1.24	1.34
3	O	36	VAL	CA-C	5.39	1.67	1.52
1	K	19	MET	CA-CB	-5.38	1.42	1.53
2	N	316	MET	C-N	-5.38	1.24	1.34
1	I	19	MET	CA-CB	-5.37	1.42	1.53
4	H	76	GLY	N-CA	5.36	1.54	1.46
1	A	19	MET	CA-CB	-5.36	1.42	1.53
1	J	19	MET	CA-CB	-5.36	1.42	1.53
1	B	19	MET	CA-CB	-5.36	1.42	1.53
1	C	19	MET	CA-CB	-5.35	1.42	1.53
2	M	289	THR	C-N	5.34	1.46	1.34
3	O	28	LEU	C-O	5.34	1.33	1.23
2	D	289	THR	C-N	5.34	1.46	1.34
2	N	289	THR	C-N	5.34	1.46	1.34
1	I	352	PRO	CA-CB	-5.30	1.43	1.53
2	F	316	MET	C-N	-5.29	1.24	1.34
1	J	352	PRO	CA-CB	-5.29	1.43	1.53
2	E	289	THR	C-N	5.29	1.46	1.34
2	F	289	THR	C-N	5.29	1.46	1.34
2	M	316	MET	C-N	-5.29	1.24	1.34
3	G	15	ARG	C-O	5.28	1.33	1.23
3	O	7	THR	N-CA	5.25	1.56	1.46
1	A	352	PRO	CA-CB	-5.25	1.43	1.53
3	G	28	LEU	C-O	5.24	1.33	1.23
1	K	352	PRO	CA-CB	-5.24	1.43	1.53
1	B	352	PRO	CA-CB	-5.23	1.43	1.53
3	O	138	ILE	CA-C	-5.23	1.39	1.52
3	O	196	ARG	C-O	5.22	1.33	1.23
4	P	29	ALA	CA-CB	-5.22	1.41	1.52
3	G	7	THR	N-CA	5.22	1.56	1.46
3	O	49	ALA	CA-C	-5.20	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	143	THR	N-CA	5.20	1.56	1.46
3	O	153	GLU	N-CA	5.18	1.56	1.46
3	G	162	ASN	C-O	5.18	1.33	1.23
4	H	29	ALA	CA-CB	-5.18	1.41	1.52
3	G	153	GLU	N-CA	5.17	1.56	1.46
3	G	200	LYS	CA-C	5.17	1.66	1.52
3	G	49	ALA	CA-C	-5.16	1.39	1.52
3	G	201	ILE	C-O	5.16	1.33	1.23
2	D	316	MET	C-N	-5.16	1.24	1.34
3	G	196	ARG	C-O	5.15	1.33	1.23
3	O	165	GLU	C-O	5.15	1.33	1.23
3	G	37	ALA	C-O	5.15	1.33	1.23
3	O	15	ARG	C-O	5.14	1.33	1.23
3	G	36	VAL	C-O	5.14	1.33	1.23
3	G	139	ARG	CA-CB	5.12	1.65	1.53
3	O	162	ASN	C-O	5.12	1.33	1.23
3	O	201	ILE	C-O	5.12	1.33	1.23
3	O	143	THR	N-CA	5.11	1.56	1.46
4	H	76	GLY	CA-C	5.10	1.60	1.51
3	O	200	LYS	CA-C	5.10	1.66	1.52
3	G	22	GLN	C-N	5.10	1.45	1.34
3	G	165	GLU	C-O	5.10	1.33	1.23
3	O	36	VAL	CA-CB	5.09	1.65	1.54
1	C	198	LYS	C-N	5.09	1.45	1.34
1	I	70	PRO	CA-C	5.08	1.63	1.52
1	C	352	PRO	CA-CB	-5.08	1.43	1.53
3	O	36	VAL	C-O	5.08	1.32	1.23
3	O	165	GLU	N-CA	5.07	1.56	1.46
3	O	160	ARG	C-O	5.06	1.32	1.23
3	O	22	GLN	C-N	5.06	1.45	1.34
3	G	138	ILE	CA-C	-5.05	1.39	1.52
3	O	37	ALA	C-O	5.05	1.32	1.23
3	O	132	ARG	C-O	5.04	1.32	1.23
3	G	36	VAL	CA-CB	5.03	1.65	1.54
3	G	50	ARG	CA-C	5.01	1.66	1.52
2	M	80	ALA	CA-C	5.01	1.66	1.52
3	G	26	ASP	C-O	5.00	1.32	1.23

All (255) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	325	ASP	O-C-N	-39.90	58.87	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	325	ASP	O-C-N	-39.90	58.87	122.70
1	A	325	ASP	O-C-N	-39.88	58.90	122.70
1	C	325	ASP	O-C-N	-39.88	58.90	122.70
1	B	325	ASP	O-C-N	-39.85	58.94	122.70
1	K	325	ASP	O-C-N	-39.85	58.94	122.70
1	K	70	PRO	C-N-CA	-33.48	37.99	121.70
1	K	70	PRO	CA-C-N	-26.39	59.13	117.20
4	P	85	ASP	CA-C-N	-23.16	66.25	117.20
1	K	70	PRO	O-C-N	22.93	159.40	122.70
1	J	429	SER	O-C-N	-19.52	91.47	122.70
4	P	85	ASP	O-C-N	19.35	153.66	122.70
1	C	325	ASP	C-N-CA	-18.31	75.92	121.70
1	A	325	ASP	C-N-CA	-18.28	76.01	121.70
1	K	325	ASP	C-N-CA	-18.25	76.08	121.70
1	B	325	ASP	C-N-CA	-18.22	76.14	121.70
1	J	325	ASP	C-N-CA	-18.22	76.16	121.70
1	I	325	ASP	C-N-CA	-18.18	76.25	121.70
1	A	429	SER	O-C-N	-17.37	94.90	122.70
4	P	77	LEU	C-N-CA	-15.81	82.18	121.70
2	D	316	MET	O-C-N	-15.67	91.32	121.10
2	L	316	MET	O-C-N	-15.63	91.40	121.10
2	E	316	MET	O-C-N	-15.61	91.45	121.10
2	F	316	MET	O-C-N	-15.57	91.52	121.10
4	P	85	ASP	CA-C-O	-15.57	87.40	120.10
2	N	316	MET	O-C-N	-15.55	91.55	121.10
2	M	316	MET	O-C-N	-15.55	91.56	121.10
1	I	325	ASP	CA-C-N	15.10	150.43	117.20
1	B	325	ASP	CA-C-N	15.08	150.38	117.20
1	J	325	ASP	CA-C-N	15.07	150.36	117.20
1	A	325	ASP	CA-C-N	15.00	150.20	117.20
1	C	325	ASP	CA-C-N	15.00	150.20	117.20
1	K	325	ASP	CA-C-N	14.98	150.16	117.20
1	I	429	SER	CA-C-N	-14.05	86.30	117.20
4	H	77	LEU	C-N-CA	-13.83	87.13	121.70
4	P	74	ILE	O-C-N	-13.23	101.54	122.70
1	I	429	SER	O-C-N	12.86	143.27	122.70
1	I	198	LYS	O-C-N	12.68	143.00	122.70
1	A	429	SER	CA-C-N	12.13	143.89	117.20
1	J	429	SER	CA-C-N	11.33	142.12	117.20
1	I	198	LYS	CA-C-N	-10.96	93.09	117.20
1	I	429	SER	C-N-CA	-10.82	94.66	121.70
3	O	47	MET	N-CA-C	10.64	139.72	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	47	MET	N-CA-C	10.62	139.69	111.00
2	L	80	ALA	C-N-CA	10.52	148.01	121.70
3	O	139	ARG	N-CA-C	-10.46	82.76	111.00
3	G	139	ARG	N-CA-C	-10.45	82.79	111.00
1	A	429	SER	C-N-CA	10.08	146.89	121.70
4	P	76	GLY	C-N-CA	10.04	146.80	121.70
3	O	6	PRO	C-N-CA	-9.82	97.16	121.70
3	G	6	PRO	C-N-CA	-9.73	97.36	121.70
3	G	6	PRO	N-CA-CB	9.71	114.95	103.30
4	P	77	LEU	CA-C-N	9.67	138.48	117.20
2	D	316	MET	CA-C-N	9.47	143.63	117.10
2	L	316	MET	CA-C-N	9.46	143.58	117.10
2	N	316	MET	CA-C-N	9.46	143.58	117.10
2	E	316	MET	CA-C-N	9.45	143.57	117.10
2	F	316	MET	CA-C-N	9.45	143.55	117.10
2	M	316	MET	CA-C-N	9.44	143.52	117.10
3	O	6	PRO	N-CA-CB	9.41	114.60	103.30
2	L	80	ALA	CA-C-N	9.41	137.90	117.20
3	O	9	MET	C-N-CA	-9.37	98.29	121.70
3	G	9	MET	C-N-CA	-9.36	98.29	121.70
3	O	49	ALA	C-N-CA	-9.15	98.83	121.70
3	G	49	ALA	C-N-CA	-9.12	98.91	121.70
4	P	76	GLY	CA-C-N	8.87	136.72	117.20
1	I	70	PRO	N-CA-C	-8.86	89.06	112.10
4	P	74	ILE	CA-C-N	8.81	136.57	117.20
1	I	63	PRO	N-CA-CB	8.73	113.77	103.30
1	K	63	PRO	N-CA-CB	8.68	113.71	103.30
1	C	63	PRO	N-CA-CB	8.67	113.70	103.30
3	O	47	MET	C-N-CA	-8.57	100.28	121.70
1	B	63	PRO	N-CA-CB	8.57	113.58	103.30
3	G	47	MET	C-N-CA	-8.56	100.30	121.70
1	J	63	PRO	N-CA-CB	8.55	113.56	103.30
4	H	77	LEU	CA-C-N	8.54	135.99	117.20
1	A	63	PRO	N-CA-CB	8.53	113.54	103.30
4	P	75	ALA	N-CA-C	8.52	134.01	111.00
3	G	187	GLU	N-CA-C	8.43	133.75	111.00
3	O	187	GLU	N-CA-C	8.35	133.53	111.00
4	H	74	ILE	O-C-N	-8.32	109.38	122.70
3	O	31	LYS	CA-C-N	-8.28	98.98	117.20
3	G	31	LYS	CA-C-N	-8.28	98.98	117.20
1	J	429	SER	C-N-CA	8.24	142.31	121.70
1	I	198	LYS	C-N-CA	-8.11	101.42	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	76	GLY	C-N-CA	8.06	141.86	121.70
3	O	186	ARG	C-N-CA	-7.87	102.03	121.70
3	O	203	ALA	N-CA-C	-7.81	89.92	111.00
3	G	203	ALA	N-CA-C	-7.79	89.96	111.00
3	G	186	ARG	C-N-CA	-7.65	102.58	121.70
3	G	167	VAL	O-C-N	-7.49	110.71	122.70
3	O	167	VAL	O-C-N	-7.47	110.75	122.70
3	O	31	LYS	O-C-N	7.34	134.45	122.70
3	G	31	LYS	O-C-N	7.29	134.37	122.70
3	O	167	VAL	C-N-CA	-7.28	103.51	121.70
3	G	167	VAL	C-N-CA	-7.26	103.55	121.70
2	L	289	THR	O-C-N	-7.25	111.11	122.70
2	D	289	THR	O-C-N	-7.20	111.17	122.70
3	G	7	THR	C-N-CA	-7.19	103.72	121.70
2	E	289	THR	O-C-N	-7.17	111.23	122.70
2	N	289	THR	O-C-N	-7.16	111.25	122.70
2	M	289	THR	O-C-N	-7.15	111.26	122.70
4	P	76	GLY	CA-C-O	-7.14	107.74	120.60
3	O	7	THR	C-N-CA	-7.13	103.86	121.70
3	G	153	GLU	N-CA-C	7.08	130.13	111.00
3	O	30	LYS	C-N-CA	7.08	139.41	121.70
2	F	289	THR	O-C-N	-7.08	111.37	122.70
3	O	133	TYR	N-CA-C	-7.08	91.89	111.00
3	G	30	LYS	C-N-CA	7.08	139.39	121.70
3	O	170	PRO	N-CA-CB	7.07	111.79	103.30
3	G	133	TYR	N-CA-C	-7.06	91.94	111.00
3	G	170	PRO	N-CA-CB	7.04	111.75	103.30
3	O	153	GLU	N-CA-C	7.02	129.96	111.00
4	H	76	GLY	CA-C-N	7.01	132.63	117.20
3	O	157	THR	N-CA-C	-7.00	92.09	111.00
3	G	157	THR	N-CA-C	-6.99	92.12	111.00
3	O	182	VAL	O-C-N	6.97	133.85	122.70
3	G	202	GLU	CA-C-N	-6.96	101.89	117.20
3	O	202	GLU	CA-C-N	-6.92	101.98	117.20
3	G	156	LYS	N-CA-C	6.90	129.63	111.00
3	O	156	LYS	N-CA-C	6.90	129.63	111.00
3	G	151	GLY	N-CA-C	-6.88	95.90	113.10
4	H	75	ALA	N-CA-C	6.86	129.51	111.00
3	O	151	GLY	N-CA-C	-6.84	96.00	113.10
3	G	182	VAL	O-C-N	6.81	133.60	122.70
4	P	65	GLY	N-CA-C	-6.76	96.20	113.10
1	C	12	PRO	N-CA-CB	6.75	111.39	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	167	VAL	CA-C-N	6.74	132.03	117.20
2	L	360	ARG	N-CA-C	-6.73	92.83	111.00
3	G	12	LEU	N-CA-C	-6.70	92.91	111.00
3	O	167	VAL	CA-C-N	6.69	131.92	117.20
1	K	12	PRO	N-CA-CB	6.67	111.31	103.30
3	O	12	LEU	N-CA-C	-6.64	93.07	111.00
1	B	12	PRO	N-CA-CB	6.62	111.24	103.30
1	A	12	PRO	N-CA-CB	6.61	111.23	103.30
1	J	12	PRO	N-CA-CB	6.60	111.22	103.30
2	L	81	ARG	CA-C-N	6.59	131.70	117.20
1	I	12	PRO	N-CA-CB	6.58	111.20	103.30
3	G	49	ALA	CA-C-N	-6.53	102.83	117.20
3	O	49	ALA	CA-C-N	-6.50	102.89	117.20
3	G	154	ILE	N-CA-C	-6.47	93.52	111.00
3	G	156	LYS	C-N-CA	-6.47	105.53	121.70
2	D	289	THR	CA-C-N	6.46	131.42	117.20
2	E	289	THR	CA-C-N	6.46	131.41	117.20
3	O	156	LYS	C-N-CA	-6.45	105.58	121.70
1	I	143	PHE	N-CA-C	6.44	128.38	111.00
2	L	359	SER	N-CA-C	-6.43	93.63	111.00
3	O	154	ILE	N-CA-C	-6.43	93.63	111.00
3	G	196	ARG	CB-CA-C	6.43	123.26	110.40
2	L	289	THR	CA-C-N	6.42	131.33	117.20
2	N	289	THR	CA-C-N	6.42	131.32	117.20
3	O	196	ARG	N-CA-CB	-6.41	99.06	110.60
3	G	196	ARG	N-CA-CB	-6.39	99.09	110.60
1	C	229	PRO	N-CA-CB	6.39	110.97	103.30
1	C	143	PHE	N-CA-C	6.38	128.22	111.00
1	J	143	PHE	N-CA-C	6.38	128.22	111.00
1	K	143	PHE	N-CA-C	6.38	128.22	111.00
2	M	289	THR	CA-C-N	6.37	131.22	117.20
3	O	196	ARG	CB-CA-C	6.37	123.14	110.40
1	B	143	PHE	N-CA-C	6.37	128.20	111.00
1	C	198	LYS	O-C-N	-6.36	112.53	122.70
1	I	69	LEU	O-C-N	6.35	133.16	121.10
4	P	77	LEU	O-C-N	-6.34	112.55	122.70
1	I	229	PRO	N-CA-CB	6.34	110.91	103.30
2	F	289	THR	CA-C-N	6.33	131.14	117.20
1	A	143	PHE	N-CA-C	6.28	127.94	111.00
1	B	229	PRO	N-CA-CB	6.28	110.83	103.30
1	J	229	PRO	N-CA-CB	6.27	110.82	103.30
3	G	199	GLY	N-CA-C	-6.26	97.45	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	199	GLY	N-CA-C	-6.25	97.48	113.10
4	P	64	ARG	N-CA-C	-6.24	94.14	111.00
1	K	229	PRO	N-CA-CB	6.23	110.78	103.30
2	D	359	SER	N-CA-C	-6.22	94.19	111.00
2	L	80	ALA	O-C-N	-6.21	112.76	122.70
1	J	70	PRO	N-CA-C	-6.13	96.16	112.10
3	O	21	ALA	O-C-N	6.11	132.48	122.70
1	A	229	PRO	N-CA-CB	6.09	110.61	103.30
3	G	21	ALA	O-C-N	6.05	132.37	122.70
2	F	17	PRO	N-CA-CB	6.01	110.51	103.30
2	E	17	PRO	N-CA-CB	5.98	110.48	103.30
2	D	17	PRO	N-CA-CB	5.97	110.47	103.30
3	G	194	LEU	N-CA-C	5.96	127.09	111.00
3	O	194	LEU	N-CA-C	5.94	127.03	111.00
2	E	81	ARG	N-CA-C	5.93	127.00	111.00
2	D	284	PRO	N-CA-CB	5.92	110.41	103.30
3	O	149	LYS	N-CA-C	-5.92	95.03	111.00
2	L	284	PRO	N-CA-CB	5.91	110.39	103.30
2	N	284	PRO	N-CA-CB	5.91	110.39	103.30
2	N	351	PRO	N-CA-CB	5.91	110.39	103.30
2	L	17	PRO	N-CA-CB	5.90	110.38	103.30
2	D	81	ARG	N-CA-C	5.88	126.88	111.00
2	N	17	PRO	N-CA-CB	5.88	110.36	103.30
3	G	149	LYS	N-CA-C	-5.88	95.13	111.00
2	M	351	PRO	N-CA-CB	5.87	110.34	103.30
2	M	17	PRO	N-CA-CB	5.87	110.34	103.30
3	G	188	ARG	N-CA-CB	5.86	121.14	110.60
2	E	284	PRO	N-CA-CB	5.85	110.32	103.30
2	D	351	PRO	N-CA-CB	5.83	110.30	103.30
2	M	81	ARG	N-CA-C	5.82	126.72	111.00
2	M	284	PRO	N-CA-CB	5.80	110.26	103.30
1	J	557	GLU	O-C-N	-5.80	113.42	122.70
2	F	284	PRO	N-CA-CB	5.80	110.26	103.30
2	L	351	PRO	N-CA-CB	5.79	110.25	103.30
3	O	21	ALA	CB-CA-C	-5.77	101.44	110.10
3	O	136	ALA	N-CA-C	-5.76	95.45	111.00
1	C	557	GLU	O-C-N	-5.76	113.49	122.70
1	B	557	GLU	O-C-N	-5.75	113.51	122.70
3	G	21	ALA	CB-CA-C	-5.74	101.48	110.10
2	E	351	PRO	N-CA-CB	5.74	110.18	103.30
3	O	188	ARG	N-CA-CB	5.73	120.92	110.60
1	K	557	GLU	O-C-N	-5.71	113.57	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	351	PRO	N-CA-CB	5.71	110.15	103.30
1	I	557	GLU	O-C-N	-5.70	113.58	122.70
1	A	557	GLU	O-C-N	-5.70	113.59	122.70
3	G	142	ASN	N-CA-C	-5.67	95.69	111.00
3	O	47	MET	N-CA-CB	-5.66	100.41	110.60
3	G	47	MET	N-CA-CB	-5.65	100.42	110.60
3	G	136	ALA	N-CA-C	-5.65	95.74	111.00
1	C	244	TRP	N-CA-C	5.64	126.24	111.00
4	H	76	GLY	CA-C-O	-5.64	110.46	120.60
1	B	244	TRP	N-CA-C	5.62	126.18	111.00
4	H	77	LEU	O-C-N	-5.62	113.71	122.70
3	O	142	ASN	N-CA-C	-5.60	95.89	111.00
1	K	244	TRP	N-CA-C	5.53	125.94	111.00
1	J	244	TRP	N-CA-C	5.53	125.93	111.00
1	I	244	TRP	N-CA-C	5.51	125.88	111.00
4	H	74	ILE	CA-C-N	5.48	129.26	117.20
3	G	47	MET	CA-C-O	5.46	131.57	120.10
2	D	360	ARG	N-CA-C	-5.46	96.27	111.00
3	G	174	ALA	C-N-CA	-5.42	108.14	121.70
4	P	35	THR	CB-CA-C	-5.41	96.99	111.60
4	H	35	THR	CB-CA-C	-5.40	97.01	111.60
3	O	47	MET	CA-C-O	5.38	131.40	120.10
3	O	155	LYS	C-N-CA	-5.37	108.28	121.70
3	O	174	ALA	C-N-CA	-5.36	108.31	121.70
3	O	140	VAL	N-CA-C	5.35	125.45	111.00
4	P	75	ALA	C-N-CA	5.35	133.54	122.30
3	G	155	LYS	C-N-CA	-5.32	108.39	121.70
3	G	140	VAL	N-CA-C	5.32	125.37	111.00
4	P	77	LEU	CA-C-O	-5.31	108.95	120.10
1	A	70	PRO	N-CA-C	-5.30	98.31	112.10
3	O	171	GLY	N-CA-C	-5.21	100.06	113.10
3	G	31	LYS	CB-CA-C	-5.21	99.98	110.40
3	O	31	LYS	CB-CA-C	-5.18	100.05	110.40
2	L	80	ALA	CA-C-O	-5.14	109.30	120.10
3	G	171	GLY	N-CA-C	-5.13	100.27	113.10
3	O	137	LEU	O-C-N	-5.11	114.52	122.70
3	O	156	LYS	CA-C-N	5.09	128.40	117.20
3	G	156	LYS	CA-C-N	5.08	128.37	117.20
2	E	79	VAL	O-C-N	-5.08	114.58	122.70
2	D	79	VAL	CA-C-N	-5.06	106.06	117.20
3	O	21	ALA	CA-C-N	-5.05	106.08	117.20
3	G	21	ALA	CA-C-N	-5.03	106.13	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	47	MET	CB-CA-C	-5.01	100.38	110.40
3	G	47	MET	CB-CA-C	-5.01	100.39	110.40

There are no chirality outliers.

All (55) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	178	GLY	Peptide
1	A	210	ARG	Mainchain
1	A	297	ALA	Mainchain
1	A	325	ASP	Mainchain
1	A	557	GLU	Mainchain
1	B	178	GLY	Peptide
1	B	210	ARG	Mainchain
1	B	297	ALA	Mainchain
1	B	325	ASP	Mainchain
1	B	557	GLU	Mainchain
1	C	178	GLY	Peptide
1	C	198	LYS	Mainchain
1	C	210	ARG	Mainchain
1	C	297	ALA	Mainchain
1	C	325	ASP	Mainchain
1	C	557	GLU	Mainchain
2	D	316	MET	Mainchain
2	D	427	GLN	Peptide
2	D	79	VAL	Mainchain
2	E	316	MET	Mainchain
2	E	427	GLN	Peptide
2	E	79	VAL	Mainchain
2	F	316	MET	Mainchain
2	F	427	GLN	Peptide
4	H	39	ARG	Peptide
4	H	82	GLN	Peptide
1	I	178	GLY	Peptide
1	I	210	ARG	Mainchain
1	I	297	ALA	Mainchain
1	I	325	ASP	Mainchain
1	I	429	SER	Mainchain
1	I	557	GLU	Mainchain
1	J	178	GLY	Peptide
1	J	210	ARG	Mainchain
1	J	297	ALA	Mainchain

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Mol	Chain	Res	Type	Group
1	J	325	ASP	Mainchain
1	J	429	SER	Mainchain
1	J	557	GLU	Mainchain
1	K	178	GLY	Peptide
1	K	210	ARG	Mainchain
1	K	297	ALA	Mainchain
1	K	325	ASP	Mainchain
1	K	557	GLU	Mainchain
1	K	70	PRO	Mainchain
2	L	316	MET	Mainchain
2	L	427	GLN	Peptide
2	L	79	VAL	Mainchain
2	M	316	MET	Mainchain
2	M	427	GLN	Peptide
2	M	79	VAL	Mainchain
2	N	316	MET	Mainchain
2	N	427	GLN	Peptide
2	N	79	VAL	Mainchain
4	P	39	ARG	Peptide
4	P	82	GLN	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2752	0	1302	87	0
1	B	2752	0	1303	71	0
1	C	2752	0	1303	98	0
1	I	2752	0	1301	134	0
1	J	2752	0	1303	52	3
1	K	2752	0	1303	91	0
2	D	2212	0	1009	73	0
2	E	2212	0	1009	56	0
2	F	2212	0	1009	78	0
2	L	2212	0	1009	94	0
2	M	2212	0	1009	50	3

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	N	2212	0	1009	78	0
3	G	639	0	299	133	0
3	O	639	0	299	135	0
4	H	509	0	255	22	0
4	P	509	0	254	18	0
All	All	32080	0	14976	1006	3

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 21.

All (1006) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:O:142:ASN:CB	3:O:142:ASN:CA	1.75	1.64
3:O:189:GLU:CA	3:O:189:GLU:CB	1.76	1.64
3:G:205:GLU:CA	3:G:205:GLU:CB	1.78	1.62
1:K:52:TYR:CA	1:K:295:PRO:CB	1.79	1.59
3:O:52:ALA:CB	3:O:52:ALA:CA	1.76	1.59
1:B:24:MET:CB	2:E:66:LEU:CA	1.74	1.58
3:O:205:GLU:CB	3:O:205:GLU:CA	1.78	1.57
3:G:189:GLU:CB	3:G:189:GLU:CA	1.76	1.57
1:B:471:VAL:CB	4:H:98:ILE:CB	1.79	1.57
3:G:52:ALA:CB	3:G:52:ALA:CA	1.75	1.57
2:D:359:SER:CB	2:D:362:MET:CB	1.78	1.56
3:O:163:ALA:C	3:O:163:ALA:CA	1.74	1.55
3:G:163:ALA:CA	3:G:163:ALA:C	1.74	1.55
3:G:142:ASN:CB	3:G:142:ASN:CA	1.75	1.54
1:I:71:LEU:CB	1:I:188:PRO:HA	1.31	1.54
1:C:52:TYR:HA	1:C:295:PRO:CB	1.16	1.54
2:N:140:VAL:CB	2:N:435:SER:CB	1.76	1.54
3:G:7:THR:CB	3:G:7:THR:CA	1.86	1.54
3:O:31:LYS:N	3:O:31:LYS:CA	1.71	1.54
1:C:52:TYR:CA	1:C:295:PRO:CB	1.85	1.53
1:I:43:ASP:C	2:L:69:ALA:CB	1.76	1.53
3:G:194:LEU:C	3:G:194:LEU:CA	1.75	1.52
1:A:71:LEU:CB	1:A:188:PRO:HA	1.35	1.52
3:O:27:LEU:CB	3:O:27:LEU:CA	1.87	1.51
3:O:194:LEU:C	3:O:194:LEU:CA	1.74	1.51
3:O:4:VAL:C	3:O:4:VAL:CA	1.78	1.51
3:O:7:THR:CB	3:O:7:THR:CA	1.86	1.51
3:G:31:LYS:CA	3:G:31:LYS:N	1.70	1.51
3:G:27:LEU:CA	3:G:27:LEU:CB	1.87	1.50
1:C:352:PRO:CB	2:F:269:GLU:HA	1.41	1.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:G:167:VAL:C	3:G:167:VAL:CA	1.81	1.49
3:G:4:VAL:C	3:G:4:VAL:CA	1.78	1.49
3:O:167:VAL:C	3:O:167:VAL:CA	1.81	1.49
1:I:44:GLY:N	2:L:69:ALA:CB	1.70	1.48
1:I:25:TYR:N	2:L:66:LEU:H	1.12	1.47
3:O:196:ARG:C	3:O:196:ARG:CA	1.84	1.46
1:B:24:MET:CB	2:E:66:LEU:HA	0.97	1.44
3:G:196:ARG:CA	3:G:196:ARG:C	1.84	1.42
4:H:65:GLY:HA3	4:H:66:ARG:CB	1.16	1.41
1:B:9:ILE:CB	2:D:50:VAL:O	1.66	1.40
2:L:359:SER:CB	2:L:362:MET:CB	1.97	1.39
1:I:43:ASP:C	2:L:69:ALA:HB2	1.33	1.38
1:C:25:TYR:CB	2:F:65:GLY:HA2	1.55	1.37
1:I:25:TYR:H	2:L:66:LEU:N	1.23	1.37
3:G:44:ARG:O	3:G:47:MET:CB	1.71	1.36
4:H:65:GLY:CA	4:H:66:ARG:CB	2.04	1.35
3:O:44:ARG:O	3:O:47:MET:CB	1.72	1.34
1:C:419:PHE:O	1:C:496:GLN:CA	1.73	1.34
1:A:11:GLY:HA3	2:F:50:VAL:O	1.17	1.34
1:K:52:TYR:HA	1:K:295:PRO:CB	0.87	1.34
1:I:11:GLY:CA	2:N:50:VAL:H	1.42	1.33
1:J:9:ILE:CB	2:L:50:VAL:O	1.78	1.32
1:C:419:PHE:O	1:C:496:GLN:HA	1.25	1.30
1:C:52:TYR:CB	1:C:295:PRO:CB	2.10	1.29
1:K:259:GLY:O	2:M:296:GLU:C	1.67	1.29
1:I:266:LEU:C	2:N:124:ARG:CB	1.99	1.29
1:K:419:PHE:O	1:K:496:GLN:CA	1.79	1.28
1:I:267:VAL:N	2:N:124:ARG:CB	1.98	1.27
1:K:44:GLY:HA2	2:N:69:ALA:CB	1.63	1.27
1:I:44:GLY:CA	2:L:69:ALA:CB	2.12	1.26
1:I:11:GLY:HA3	2:N:50:VAL:C	1.55	1.26
1:I:224:ALA:CB	1:I:405:ALA:HB3	1.65	1.25
1:I:24:MET:HA	2:L:66:LEU:CA	1.65	1.25
1:C:224:ALA:CB	1:C:405:ALA:HB3	1.65	1.25
1:J:224:ALA:CB	1:J:405:ALA:HB3	1.65	1.24
1:B:224:ALA:CB	1:B:405:ALA:HB3	1.65	1.24
1:K:69:LEU:CB	1:K:72:ALA:HB3	1.66	1.24
1:A:224:ALA:CB	1:A:405:ALA:HB3	1.65	1.24
1:K:224:ALA:CB	1:K:405:ALA:HB3	1.66	1.23
2:M:140:VAL:CB	2:M:435:SER:CB	2.16	1.23
1:K:419:PHE:O	1:K:497:GLN:N	1.70	1.22
4:H:84:HIS:O	4:H:86:VAL:N	1.72	1.22

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:71:LEU:CB	1:I:188:PRO:CA	2.18	1.22
1:C:419:PHE:O	1:C:496:GLN:CB	1.86	1.21
1:I:11:GLY:CA	2:N:50:VAL:N	2.03	1.20
1:I:44:GLY:CA	2:L:69:ALA:HB1	1.68	1.20
1:I:11:GLY:HA3	2:N:50:VAL:O	1.40	1.20
1:K:419:PHE:O	1:K:496:GLN:HA	1.12	1.19
2:F:426:GLY:O	1:K:125:PRO:C	1.80	1.18
1:I:11:GLY:HA3	2:N:50:VAL:CA	1.72	1.17
1:I:43:ASP:C	2:L:69:ALA:HB3	1.66	1.16
1:B:10:ALA:O	2:D:50:VAL:N	1.77	1.16
1:C:352:PRO:CB	2:F:269:GLU:CA	2.23	1.16
1:B:11:GLY:HA3	2:D:49:GLU:CB	1.75	1.15
1:B:263:THR:CB	2:D:125:ARG:N	2.10	1.15
1:I:266:LEU:CB	2:N:124:ARG:CB	2.25	1.14
1:A:71:LEU:CB	1:A:188:PRO:CA	2.25	1.14
1:B:10:ALA:H	2:D:50:VAL:CB	1.60	1.12
1:A:10:ALA:O	2:F:50:VAL:CB	1.98	1.12
1:I:44:GLY:N	2:L:69:ALA:HB1	1.43	1.11
1:C:25:TYR:H	2:F:66:LEU:N	1.48	1.11
1:K:44:GLY:HA2	2:N:69:ALA:HB3	1.25	1.11
1:A:44:GLY:HA2	2:D:69:ALA:CB	1.80	1.10
1:A:266:LEU:CB	2:F:124:ARG:CB	2.29	1.10
1:I:44:GLY:HA2	2:L:69:ALA:CB	1.78	1.10
1:I:11:GLY:HA3	2:N:50:VAL:N	1.65	1.10
1:C:189:VAL:CB	1:C:305:VAL:HA	1.81	1.10
1:C:25:TYR:N	2:F:66:LEU:H	1.49	1.09
1:I:43:ASP:O	2:L:69:ALA:HB3	1.49	1.09
1:I:24:MET:CA	2:L:66:LEU:HA	1.81	1.09
1:C:44:GLY:HA2	2:F:69:ALA:CB	1.83	1.08
2:M:359:SER:CB	2:M:362:MET:CB	2.31	1.08
4:H:62:LEU:O	4:H:63:MET:O	1.69	1.08
1:B:25:TYR:O	2:E:65:GLY:HA2	1.53	1.07
4:P:75:ALA:HB2	4:P:85:ASP:O	1.54	1.07
1:A:44:GLY:HA2	2:D:69:ALA:HB3	1.32	1.07
2:D:149:LYS:O	2:D:334:GLU:N	1.87	1.07
3:O:176:ILE:O	3:O:179:ILE:CB	2.03	1.06
2:F:149:LYS:O	2:F:334:GLU:N	1.87	1.06
2:N:149:LYS:O	2:N:334:GLU:N	1.87	1.06
3:G:176:ILE:O	3:G:179:ILE:CB	2.03	1.06
2:L:149:LYS:O	2:L:334:GLU:N	1.87	1.06
2:E:149:LYS:O	2:E:334:GLU:N	1.87	1.06
1:I:11:GLY:CA	2:N:50:VAL:O	2.02	1.06

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:263:THR:CB	2:D:124:ARG:C	2.25	1.05
1:I:259:GLY:N	2:N:296:GLU:CA	2.06	1.05
2:M:149:LYS:O	2:M:334:GLU:N	1.87	1.05
1:B:9:ILE:HA	2:D:50:VAL:CB	1.87	1.04
1:A:11:GLY:CA	2:F:50:VAL:O	2.05	1.04
1:A:352:PRO:CB	2:D:272:ALA:HB3	1.88	1.04
1:I:44:GLY:CA	2:L:69:ALA:HB3	1.83	1.03
1:A:69:LEU:CB	1:A:71:LEU:C	2.26	1.03
1:A:44:GLY:CA	2:D:69:ALA:CB	2.35	1.03
3:O:27:LEU:CB	3:O:163:ALA:HB2	1.87	1.03
1:B:11:GLY:HA3	2:D:49:GLU:CA	1.88	1.03
1:A:44:GLY:N	2:D:69:ALA:CB	2.22	1.03
1:I:11:GLY:HA2	2:N:50:VAL:N	1.66	1.02
1:C:224:ALA:HB1	1:C:405:ALA:HB3	1.41	1.02
1:I:224:ALA:HB1	1:I:405:ALA:HB3	1.41	1.01
1:A:224:ALA:HB1	1:A:405:ALA:HB3	1.41	1.01
4:H:76:GLY:O	4:H:80:ALA:HB3	1.59	1.01
1:I:71:LEU:CB	1:I:189:VAL:H	1.74	1.01
1:K:44:GLY:CA	2:N:69:ALA:CB	2.39	1.00
1:K:224:ALA:HB1	1:K:405:ALA:HB3	1.41	1.00
1:K:259:GLY:O	2:M:296:GLU:O	1.78	1.00
1:K:52:TYR:CB	1:K:295:PRO:CB	2.38	1.00
4:P:62:LEU:O	4:P:63:MET:CB	2.07	0.99
3:O:7:THR:O	3:O:8:ARG:C	1.98	0.99
1:J:224:ALA:HB1	1:J:405:ALA:HB3	1.41	0.99
1:B:224:ALA:HB2	1:B:405:ALA:HB3	1.45	0.99
1:C:24:MET:HA	2:F:66:LEU:HA	1.45	0.99
1:C:419:PHE:C	1:C:496:GLN:HA	1.83	0.98
2:L:334:GLU:O	2:L:361:LEU:N	1.96	0.98
1:C:11:GLY:HA3	2:E:50:VAL:H	1.28	0.98
1:B:24:MET:CB	2:E:66:LEU:N	2.26	0.98
1:J:471:VAL:CB	4:P:98:ILE:O	2.12	0.98
1:B:224:ALA:HB1	1:B:405:ALA:HB3	1.42	0.97
1:I:259:GLY:N	2:N:296:GLU:HA	1.78	0.97
3:G:7:THR:O	3:G:8:ARG:C	1.98	0.97
1:I:11:GLY:HA2	2:N:50:VAL:H	0.81	0.97
1:K:25:TYR:CB	2:N:65:GLY:HA2	1.94	0.97
3:G:199:GLY:O	3:G:203:ALA:HB2	1.63	0.97
1:B:9:ILE:CB	2:D:50:VAL:C	2.32	0.97
1:I:43:ASP:CA	2:L:69:ALA:HB2	1.94	0.97
1:C:224:ALA:HB2	1:C:405:ALA:HB3	1.46	0.97
1:K:259:GLY:C	2:M:296:GLU:C	2.22	0.96

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:419:PHE:O	1:J:496:GLN:HA	1.63	0.96
1:A:69:LEU:CB	1:A:72:ALA:N	2.27	0.96
1:I:224:ALA:HB2	1:I:405:ALA:HB3	1.46	0.96
2:F:149:LYS:O	2:F:333:THR:HA	1.66	0.96
3:G:199:GLY:C	3:G:203:ALA:HB2	1.86	0.96
1:A:224:ALA:HB2	1:A:405:ALA:HB3	1.46	0.96
3:O:199:GLY:O	3:O:203:ALA:HB2	1.63	0.96
1:K:44:GLY:HA2	2:N:69:ALA:HB2	1.47	0.96
1:J:224:ALA:HB2	1:J:405:ALA:HB3	1.45	0.96
1:C:292:SER:CB	2:E:292:ALA:HB3	1.96	0.96
2:L:150:LEU:HA	2:L:335:GLY:O	1.66	0.96
1:A:11:GLY:HA3	2:F:50:VAL:C	1.86	0.95
1:I:267:VAL:N	2:N:124:ARG:CA	2.24	0.95
1:K:419:PHE:O	1:K:496:GLN:C	2.03	0.95
1:K:224:ALA:HB2	1:K:405:ALA:HB3	1.46	0.95
2:F:150:LEU:HA	2:F:335:GLY:O	1.66	0.95
1:A:69:LEU:CB	1:A:71:LEU:O	2.14	0.95
2:D:150:LEU:HA	2:D:335:GLY:O	1.67	0.95
2:N:150:LEU:HA	2:N:335:GLY:O	1.66	0.95
3:G:148:LYS:O	3:G:152:GLU:CB	2.15	0.95
2:N:149:LYS:O	2:N:333:THR:HA	1.66	0.95
1:I:259:GLY:O	2:N:296:GLU:C	2.05	0.95
1:B:11:GLY:HA3	2:D:49:GLU:HA	1.49	0.94
3:O:47:MET:O	3:O:49:ALA:N	2.00	0.94
3:O:199:GLY:C	3:O:203:ALA:HB2	1.86	0.94
1:I:25:TYR:CB	2:L:65:GLY:HA2	1.96	0.94
2:L:149:LYS:O	2:L:333:THR:HA	1.66	0.94
2:E:150:LEU:HA	2:E:335:GLY:O	1.66	0.94
2:M:150:LEU:HA	2:M:335:GLY:O	1.67	0.94
2:N:134:GLY:O	2:N:429:ASN:HA	1.68	0.94
2:D:149:LYS:O	2:D:333:THR:HA	1.66	0.94
1:C:267:VAL:O	2:E:125:ARG:HA	1.62	0.94
1:C:11:GLY:HA3	2:E:50:VAL:N	1.82	0.94
3:O:135:GLU:C	3:O:137:LEU:N	2.17	0.93
3:O:148:LYS:O	3:O:152:GLU:CB	2.15	0.93
1:A:44:GLY:CA	2:D:69:ALA:HB3	1.96	0.93
3:G:47:MET:O	3:G:49:ALA:N	2.00	0.93
2:L:149:LYS:O	2:L:333:THR:CA	2.17	0.93
2:F:426:GLY:O	1:K:125:PRO:O	1.86	0.93
4:P:86:VAL:O	4:P:88:GLY:N	2.01	0.93
2:N:149:LYS:O	2:N:333:THR:CA	2.16	0.93
4:P:77:LEU:O	4:P:78:LYS:C	1.88	0.93

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:71:LEU:CB	1:A:72:ALA:HA	1.99	0.93
4:P:75:ALA:CB	4:P:85:ASP:O	2.17	0.93
2:E:149:LYS:O	2:E:333:THR:HA	1.66	0.93
2:F:149:LYS:O	2:F:333:THR:CA	2.16	0.93
2:M:149:LYS:O	2:M:333:THR:HA	1.66	0.93
2:D:149:LYS:O	2:D:333:THR:CA	2.16	0.93
2:E:149:LYS:O	2:E:333:THR:CA	2.17	0.92
1:J:24:MET:CB	2:M:66:LEU:HA	1.99	0.92
1:I:71:LEU:CB	1:I:189:VAL:N	2.33	0.92
1:B:10:ALA:N	2:D:50:VAL:CB	2.31	0.92
3:O:48:GLU:O	3:O:51:LYS:CB	2.18	0.92
3:G:48:GLU:O	3:G:51:LYS:CB	2.18	0.91
1:A:71:LEU:CB	1:A:189:VAL:H	1.83	0.91
1:K:69:LEU:CB	1:K:72:ALA:CB	2.47	0.91
1:C:11:GLY:CA	2:E:50:VAL:H	1.82	0.91
2:M:149:LYS:O	2:M:333:THR:CA	2.17	0.91
1:C:266:LEU:CB	2:E:124:ARG:HA	1.99	0.91
2:E:359:SER:CB	2:E:362:MET:CB	2.49	0.91
4:P:84:HIS:O	4:P:86:VAL:N	2.03	0.90
1:I:43:ASP:O	2:L:69:ALA:CB	2.08	0.90
3:G:49:ALA:O	3:G:52:ALA:HB3	1.72	0.90
4:P:84:HIS:O	4:P:86:VAL:CB	2.19	0.90
3:O:141:ALA:O	3:O:145:THR:CB	2.21	0.89
1:A:44:GLY:CA	2:D:69:ALA:HB1	2.02	0.89
1:K:44:GLY:CA	2:N:69:ALA:HB2	2.03	0.89
3:O:49:ALA:O	3:O:52:ALA:HB3	1.72	0.88
4:H:76:GLY:O	4:H:80:ALA:CB	2.20	0.88
3:G:141:ALA:O	3:G:145:THR:CB	2.21	0.88
2:F:295:TYR:CB	2:F:332:ILE:CB	2.53	0.87
2:E:140:VAL:CB	2:E:435:SER:CB	2.52	0.87
1:I:44:GLY:HA2	2:L:69:ALA:HB3	1.48	0.87
2:N:295:TYR:CB	2:N:332:ILE:CB	2.53	0.87
2:M:295:TYR:CB	2:M:332:ILE:CB	2.52	0.87
3:G:135:GLU:C	3:G:137:LEU:N	2.17	0.86
2:F:359:SER:CB	2:F:362:MET:CB	2.53	0.86
1:K:10:ALA:O	2:M:50:VAL:CB	2.23	0.86
2:D:295:TYR:CB	2:D:332:ILE:CB	2.53	0.86
2:L:295:TYR:CB	2:L:332:ILE:CB	2.53	0.86
4:H:77:LEU:H	4:H:80:ALA:HB3	1.41	0.86
2:L:153:PHE:O	2:L:339:LEU:N	2.08	0.86
1:B:10:ALA:O	2:D:49:GLU:HA	1.74	0.86
2:D:134:GLY:HA2	2:D:430:ARG:O	1.76	0.86

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:419:PHE:C	1:K:496:GLN:HA	1.95	0.86
1:I:259:GLY:C	2:N:296:GLU:CA	2.44	0.86
1:I:24:MET:HA	2:L:66:LEU:HA	0.86	0.86
2:L:150:LEU:CA	2:L:335:GLY:O	2.24	0.86
1:I:12:PRO:N	2:N:49:GLU:CB	2.39	0.86
3:G:47:MET:O	3:G:48:GLU:C	2.09	0.86
2:F:153:PHE:O	2:F:339:LEU:N	2.09	0.86
2:M:153:PHE:O	2:M:339:LEU:N	2.09	0.86
1:J:263:THR:CB	2:L:125:ARG:N	2.38	0.86
2:E:295:TYR:CB	2:E:332:ILE:CB	2.53	0.86
3:G:174:ALA:O	3:G:175:GLN:C	2.09	0.85
2:F:150:LEU:CA	2:F:335:GLY:O	2.24	0.85
2:M:150:LEU:CA	2:M:335:GLY:O	2.24	0.85
1:C:260:ASN:CB	2:E:298:ALA:HB3	2.06	0.85
3:O:47:MET:O	3:O:48:GLU:C	2.09	0.85
2:N:153:PHE:O	2:N:339:LEU:N	2.09	0.85
3:O:174:ALA:O	3:O:175:GLN:C	2.09	0.85
4:H:77:LEU:N	4:H:80:ALA:HB3	1.91	0.85
2:D:150:LEU:CA	2:D:335:GLY:O	2.24	0.85
2:E:150:LEU:CA	2:E:335:GLY:O	2.24	0.85
1:C:266:LEU:C	2:E:124:ARG:CB	2.45	0.85
1:B:24:MET:CB	2:E:66:LEU:C	2.44	0.85
1:I:11:GLY:CA	2:N:50:VAL:CA	2.50	0.85
1:I:52:TYR:CB	1:I:297:ALA:HB3	2.08	0.84
3:O:199:GLY:O	3:O:203:ALA:CB	2.26	0.84
2:D:153:PHE:O	2:D:339:LEU:N	2.09	0.84
1:I:24:MET:C	2:L:66:LEU:H	1.79	0.84
1:B:10:ALA:C	2:D:50:VAL:H	1.79	0.84
2:N:150:LEU:CA	2:N:335:GLY:O	2.24	0.84
1:C:208:GLY:HA2	1:C:507:CYS:O	1.78	0.84
1:I:25:TYR:N	2:L:66:LEU:N	1.94	0.83
1:A:43:ASP:C	2:D:69:ALA:CB	2.46	0.83
1:I:24:MET:CA	2:L:66:LEU:CA	2.50	0.83
1:I:259:GLY:C	2:N:296:GLU:C	2.37	0.83
2:E:153:PHE:O	2:E:339:LEU:N	2.09	0.83
3:O:158:THR:O	3:O:161:VAL:CB	2.27	0.83
3:G:158:THR:O	3:G:161:VAL:CB	2.27	0.82
1:I:25:TYR:CA	2:L:65:GLY:HA2	2.09	0.82
1:C:18:GLY:O	1:C:19:MET:CB	2.28	0.82
3:G:199:GLY:O	3:G:203:ALA:CB	2.25	0.82
1:C:208:GLY:O	1:C:507:CYS:CB	2.28	0.82
1:I:18:GLY:O	1:I:19:MET:CB	2.27	0.82

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:189:VAL:CB	1:C:305:VAL:CA	2.58	0.81
1:I:56:SER:CB	2:N:30:GLY:N	2.43	0.81
1:B:263:THR:CB	2:D:125:ARG:CA	2.59	0.81
1:C:344:MET:CB	2:F:272:ALA:HB1	2.11	0.81
3:G:167:VAL:O	3:G:168:VAL:C	2.19	0.80
3:O:167:VAL:O	3:O:169:ILE:N	2.14	0.80
1:K:18:GLY:O	1:K:19:MET:CB	2.28	0.80
2:F:427:GLN:CB	1:K:126:GLY:HA3	2.12	0.80
1:A:259:GLY:N	2:F:296:GLU:HA	1.96	0.80
1:B:9:ILE:CA	2:D:50:VAL:CB	2.60	0.80
1:A:43:ASP:C	2:D:69:ALA:HB2	2.02	0.80
1:J:18:GLY:O	1:J:19:MET:CB	2.28	0.80
1:I:266:LEU:CA	2:N:124:ARG:CB	2.59	0.80
4:H:76:GLY:C	4:H:80:ALA:HB3	2.00	0.80
1:J:224:ALA:HB1	1:J:405:ALA:CB	2.12	0.80
3:G:167:VAL:O	3:G:169:ILE:N	2.14	0.79
1:A:224:ALA:HB1	1:A:405:ALA:CB	2.12	0.79
1:B:18:GLY:O	1:B:19:MET:CB	2.28	0.79
1:I:24:MET:CA	2:L:66:LEU:N	2.46	0.79
1:C:224:ALA:HB1	1:C:405:ALA:CB	2.12	0.79
1:B:224:ALA:HB1	1:B:405:ALA:CB	2.12	0.79
1:I:260:ASN:CB	2:N:298:ALA:O	2.30	0.79
1:K:419:PHE:C	1:K:497:GLN:H	1.86	0.79
3:G:132:ARG:N	3:G:134:ALA:HB3	1.98	0.79
1:I:224:ALA:HB1	1:I:405:ALA:CB	2.12	0.79
1:K:224:ALA:HB1	1:K:405:ALA:CB	2.13	0.79
1:A:71:LEU:CB	1:A:189:VAL:N	2.45	0.78
2:L:334:GLU:CB	2:L:361:LEU:CB	2.60	0.78
3:O:167:VAL:O	3:O:168:VAL:C	2.19	0.78
1:C:201:PRO:O	1:C:434:ALA:HB1	1.84	0.78
3:O:132:ARG:N	3:O:134:ALA:HB3	1.98	0.78
1:C:266:LEU:C	2:E:124:ARG:CA	2.50	0.78
1:B:11:GLY:CA	2:D:49:GLU:HA	2.13	0.78
1:A:18:GLY:O	1:A:19:MET:CB	2.28	0.78
1:C:259:GLY:O	2:E:297:ARG:N	2.16	0.77
3:G:28:LEU:O	3:G:31:LYS:CB	2.32	0.77
3:O:28:LEU:O	3:O:31:LYS:CB	2.32	0.77
2:L:359:SER:C	2:L:361:LEU:H	1.86	0.77
2:D:334:GLU:O	2:D:361:LEU:N	2.17	0.77
1:I:267:VAL:H	2:N:124:ARG:CA	1.97	0.77
1:I:419:PHE:CB	1:I:497:GLN:O	2.32	0.77
2:F:51:SER:O	2:F:52:GLU:CB	2.33	0.77

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:M:51:SER:O	2:M:52:GLU:CB	2.33	0.77
1:B:10:ALA:O	2:D:49:GLU:CA	2.33	0.76
1:C:224:ALA:CB	1:C:405:ALA:CB	2.58	0.76
1:C:44:GLY:HA2	2:F:69:ALA:HB1	1.67	0.76
2:L:359:SER:C	2:L:361:LEU:N	2.26	0.76
2:D:51:SER:O	2:D:52:GLU:CB	2.33	0.76
1:A:11:GLY:HA2	2:F:50:VAL:H	1.47	0.76
1:C:259:GLY:O	2:E:296:GLU:C	2.24	0.76
2:L:51:SER:O	2:L:52:GLU:CB	2.33	0.76
1:I:259:GLY:C	2:N:296:GLU:HA	2.04	0.76
1:J:263:THR:CB	2:L:125:ARG:C	2.54	0.76
1:J:419:PHE:O	1:J:496:GLN:CA	2.35	0.75
2:N:51:SER:O	2:N:52:GLU:CB	2.33	0.75
1:I:224:ALA:CB	1:I:405:ALA:CB	2.58	0.75
1:I:71:LEU:CB	1:I:72:ALA:HA	2.17	0.75
3:O:194:LEU:HA	3:O:194:LEU:C	2.04	0.75
2:E:149:LYS:CB	2:E:332:ILE:O	2.35	0.75
2:L:149:LYS:CB	2:L:332:ILE:O	2.35	0.75
1:C:25:TYR:CB	2:F:65:GLY:CA	2.51	0.75
2:F:149:LYS:CB	2:F:332:ILE:O	2.35	0.75
2:E:51:SER:O	2:E:52:GLU:CB	2.33	0.75
1:B:224:ALA:CB	1:B:405:ALA:CB	2.58	0.74
1:B:419:PHE:O	1:B:496:GLN:HA	1.87	0.74
3:G:132:ARG:C	3:G:134:ALA:N	2.37	0.74
1:I:56:SER:CB	2:N:30:GLY:O	2.35	0.74
3:O:140:VAL:O	3:O:144:GLU:CB	2.35	0.74
3:G:199:GLY:C	3:G:203:ALA:CB	2.56	0.74
3:O:199:GLY:C	3:O:203:ALA:CB	2.56	0.74
3:O:132:ARG:C	3:O:134:ALA:N	2.37	0.74
3:G:140:VAL:O	3:G:144:GLU:CB	2.35	0.73
2:N:69:ALA:O	2:N:70:THR:CB	2.36	0.73
2:M:149:LYS:CB	2:M:332:ILE:O	2.35	0.73
3:O:142:ASN:O	3:O:146:ARG:CB	2.36	0.73
3:G:142:ASN:O	3:G:146:ARG:CB	2.36	0.73
3:G:196:ARG:HA	3:G:196:ARG:C	2.05	0.73
2:N:149:LYS:CB	2:N:332:ILE:O	2.35	0.73
2:D:149:LYS:CB	2:D:332:ILE:O	2.35	0.73
3:O:45:GLU:O	3:O:46:ALA:C	2.27	0.73
2:L:69:ALA:O	2:L:70:THR:CB	2.36	0.73
3:G:45:GLU:O	3:G:46:ALA:C	2.27	0.73
1:A:224:ALA:CB	1:A:405:ALA:CB	2.58	0.73
1:B:263:THR:CB	2:D:125:ARG:C	2.58	0.73

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:69:ALA:O	2:F:70:THR:CB	2.37	0.73
1:C:292:SER:CB	2:E:292:ALA:CB	2.67	0.73
1:I:24:MET:HA	2:L:66:LEU:N	2.04	0.72
3:O:150:ILE:O	3:O:151:GLY:O	2.07	0.72
2:E:69:ALA:O	2:E:70:THR:CB	2.37	0.72
3:G:163:ALA:HA	3:G:163:ALA:C	2.04	0.72
3:G:150:ILE:O	3:G:151:GLY:O	2.08	0.72
4:H:74:ILE:O	4:H:75:ALA:O	2.07	0.72
2:D:69:ALA:O	2:D:70:THR:CB	2.36	0.72
2:N:65:GLY:O	2:N:66:LEU:CB	2.38	0.72
2:M:69:ALA:O	2:M:70:THR:CB	2.37	0.72
1:A:69:LEU:CB	1:A:72:ALA:H	1.99	0.71
3:O:135:GLU:O	3:O:136:ALA:C	2.28	0.71
1:A:44:GLY:HA2	2:D:69:ALA:HB1	1.63	0.71
3:G:4:VAL:C	3:G:4:VAL:HA	2.07	0.71
3:O:196:ARG:C	3:O:196:ARG:HA	2.05	0.71
2:N:359:SER:CB	2:N:362:MET:CB	2.68	0.71
3:G:135:GLU:O	3:G:136:ALA:C	2.28	0.71
1:B:10:ALA:O	2:D:49:GLU:C	2.29	0.71
2:F:65:GLY:O	2:F:66:LEU:CB	2.39	0.70
2:E:65:GLY:O	2:E:66:LEU:CB	2.38	0.70
1:I:225:ALA:N	1:I:405:ALA:O	2.25	0.70
1:A:225:ALA:N	1:A:405:ALA:O	2.25	0.70
2:M:65:GLY:O	2:M:66:LEU:CB	2.38	0.70
2:L:274:ARG:O	2:L:275:GLU:CB	2.37	0.70
1:C:266:LEU:O	2:E:124:ARG:CB	2.40	0.70
1:I:132:GLY:HA3	1:I:371:LEU:CB	2.22	0.70
1:B:471:VAL:CB	4:H:98:ILE:CA	2.69	0.70
1:K:225:ALA:N	1:K:405:ALA:O	2.25	0.70
2:F:274:ARG:O	2:F:275:GLU:CB	2.37	0.69
1:A:259:GLY:CA	2:F:296:GLU:HA	2.21	0.69
2:N:274:ARG:O	2:N:275:GLU:CB	2.37	0.69
2:D:65:GLY:O	2:D:66:LEU:CB	2.38	0.69
1:C:225:ALA:N	1:C:405:ALA:O	2.25	0.69
1:J:225:ALA:N	1:J:405:ALA:O	2.25	0.69
1:B:225:ALA:N	1:B:405:ALA:O	2.25	0.69
2:M:274:ARG:O	2:M:275:GLU:CB	2.37	0.69
3:O:48:GLU:C	3:O:51:LYS:H	1.97	0.69
3:O:31:LYS:N	3:O:31:LYS:HA	2.02	0.69
2:L:65:GLY:O	2:L:66:LEU:CB	2.39	0.69
3:O:197:ILE:O	3:O:200:LYS:CB	2.41	0.68
3:O:4:VAL:HA	3:O:4:VAL:C	2.07	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:G:197:ILE:O	3:G:200:LYS:CB	2.40	0.68
1:A:5:VAL:CB	1:A:18:GLY:O	2.42	0.68
1:K:5:VAL:CB	1:K:18:GLY:O	2.42	0.68
1:J:5:VAL:CB	1:J:18:GLY:O	2.42	0.68
1:B:24:MET:CB	2:E:66:LEU:H	2.06	0.68
1:I:5:VAL:CB	1:I:18:GLY:O	2.42	0.68
2:F:427:GLN:CB	1:K:126:GLY:CA	2.72	0.68
1:J:224:ALA:CB	1:J:405:ALA:CB	2.58	0.68
1:K:224:ALA:CB	1:K:405:ALA:CB	2.58	0.68
2:D:359:SER:C	2:D:361:LEU:N	2.41	0.68
3:G:48:GLU:C	3:G:51:LYS:H	1.97	0.67
2:E:274:ARG:O	2:E:275:GLU:CB	2.37	0.67
1:C:5:VAL:CB	1:C:18:GLY:O	2.42	0.67
2:F:61:GLU:HA	2:F:229:ILE:CB	2.25	0.67
3:G:194:LEU:HA	3:G:194:LEU:C	2.04	0.67
1:I:292:SER:CB	2:N:292:ALA:HB3	2.24	0.67
1:B:5:VAL:CB	1:B:18:GLY:O	2.42	0.67
3:G:151:GLY:HA2	3:G:155:LYS:CB	2.25	0.67
3:G:31:LYS:N	3:G:31:LYS:HA	2.02	0.67
2:D:274:ARG:O	2:D:275:GLU:CB	2.37	0.67
3:O:151:GLY:HA2	3:O:155:LYS:CB	2.26	0.66
1:C:352:PRO:CB	2:F:269:GLU:C	2.63	0.66
3:G:3:GLN:O	3:G:5:SER:N	2.29	0.66
4:P:86:VAL:O	4:P:89:TYR:N	2.29	0.66
1:A:71:LEU:CB	1:A:72:ALA:CA	2.74	0.66
3:O:141:ALA:HA	3:O:144:GLU:CB	2.26	0.66
1:B:24:MET:HA	2:E:67:ASP:O	1.96	0.66
3:O:3:GLN:O	3:O:5:SER:N	2.29	0.66
1:C:260:ASN:N	2:E:296:GLU:HA	2.09	0.66
1:K:189:VAL:O	1:K:304:TYR:CB	2.44	0.66
3:G:141:ALA:HA	3:G:144:GLU:CB	2.26	0.66
1:K:266:LEU:CB	2:M:124:ARG:CB	2.74	0.66
1:C:352:PRO:CB	2:F:269:GLU:O	2.44	0.65
1:A:11:GLY:CA	2:F:50:VAL:H	2.10	0.65
1:J:263:THR:CB	2:L:124:ARG:C	2.65	0.65
2:M:61:GLU:O	2:M:227:PRO:CB	2.44	0.65
2:M:149:LYS:O	2:M:333:THR:C	2.35	0.65
1:A:292:SER:CB	2:F:292:ALA:HB1	2.26	0.65
2:L:334:GLU:O	2:L:361:LEU:CB	2.44	0.65
1:K:26:ASP:O	1:K:71:LEU:N	2.30	0.65
2:N:149:LYS:O	2:N:333:THR:C	2.35	0.65
3:O:163:ALA:C	3:O:163:ALA:HA	2.04	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:149:LYS:O	2:F:333:THR:C	2.35	0.65
2:E:149:LYS:O	2:E:333:THR:C	2.35	0.65
1:K:132:GLY:HA3	1:K:371:LEU:CB	2.27	0.65
3:O:172:ILE:O	3:O:176:ILE:CB	2.45	0.64
1:I:71:LEU:CB	1:I:188:PRO:C	2.64	0.64
2:L:149:LYS:O	2:L:333:THR:C	2.35	0.64
1:I:44:GLY:HA2	2:L:69:ALA:HB1	1.53	0.64
2:F:426:GLY:O	1:K:125:PRO:CB	2.46	0.64
3:G:141:ALA:HA	3:G:145:THR:H	1.62	0.64
3:O:156:LYS:C	3:O:158:THR:N	2.44	0.64
1:B:11:GLY:CA	2:D:49:GLU:CB	2.66	0.64
1:K:11:GLY:HA3	2:M:49:GLU:CA	2.28	0.64
3:G:156:LYS:C	3:G:158:THR:N	2.44	0.64
3:O:156:LYS:O	3:O:157:THR:C	2.33	0.64
2:D:149:LYS:O	2:D:333:THR:C	2.35	0.64
1:I:25:TYR:O	2:L:65:GLY:HA2	1.97	0.64
3:G:172:ILE:O	3:G:176:ILE:CB	2.45	0.64
3:O:141:ALA:HA	3:O:145:THR:H	1.62	0.63
1:A:259:GLY:CA	2:F:296:GLU:CA	2.73	0.63
1:K:11:GLY:CA	2:M:49:GLU:HA	2.29	0.63
1:I:346:ALA:HB2	2:L:272:ALA:HB1	1.80	0.63
3:G:151:GLY:O	3:G:152:GLU:C	2.36	0.63
1:B:71:LEU:O	1:B:72:ALA:HB2	1.98	0.63
3:O:151:GLY:O	3:O:152:GLU:C	2.37	0.63
1:K:56:SER:CB	2:M:30:GLY:O	2.47	0.63
2:E:134:GLY:O	2:E:429:ASN:HA	1.97	0.63
4:H:62:LEU:O	4:H:63:MET:C	2.34	0.63
1:A:259:GLY:H	2:F:296:GLU:CA	2.11	0.63
1:A:259:GLY:N	2:F:296:GLU:CA	2.62	0.63
1:I:346:ALA:HB2	2:L:272:ALA:CB	2.29	0.63
2:N:76:VAL:O	2:N:77:GLU:CB	2.47	0.63
3:O:156:LYS:HA	3:O:159:ARG:H	1.64	0.63
3:G:18:LEU:O	3:G:21:ALA:HB3	1.99	0.63
1:I:70:PRO:CB	1:I:190:ARG:CB	2.77	0.63
2:F:76:VAL:O	2:F:77:GLU:CB	2.47	0.63
3:O:148:LYS:O	3:O:149:LYS:O	2.17	0.62
1:B:25:TYR:O	2:E:65:GLY:CA	2.40	0.62
2:E:76:VAL:O	2:E:77:GLU:CB	2.47	0.62
2:L:76:VAL:O	2:L:77:GLU:CB	2.47	0.62
1:I:267:VAL:CA	2:N:124:ARG:CB	2.74	0.62
3:G:156:LYS:HA	3:G:159:ARG:H	1.64	0.62
3:O:18:LEU:O	3:O:21:ALA:HB3	1.99	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:G:156:LYS:O	3:G:157:THR:C	2.33	0.62
3:O:135:GLU:C	3:O:137:LEU:H	2.03	0.62
1:K:25:TYR:CB	2:N:65:GLY:CA	2.74	0.62
1:I:259:GLY:O	2:N:296:GLU:O	2.18	0.62
3:O:41:GLY:O	3:O:42:LEU:C	2.38	0.61
1:K:11:GLY:HA3	2:M:49:GLU:CB	2.30	0.61
1:J:10:ALA:O	2:L:49:GLU:HA	1.99	0.61
3:G:41:GLY:O	3:G:42:LEU:C	2.38	0.61
3:O:27:LEU:CB	3:O:163:ALA:CB	2.73	0.61
2:D:76:VAL:O	2:D:77:GLU:CB	2.47	0.61
3:G:148:LYS:O	3:G:149:LYS:O	2.17	0.61
1:A:69:LEU:C	1:A:71:LEU:O	2.37	0.61
4:H:77:LEU:H	4:H:80:ALA:CB	2.12	0.61
2:E:61:GLU:O	2:E:227:PRO:CB	2.48	0.61
1:I:24:MET:CA	2:L:66:LEU:H	2.08	0.61
1:A:259:GLY:H	2:F:296:GLU:N	1.97	0.61
1:I:11:GLY:CA	2:N:50:VAL:CB	2.78	0.61
3:O:170:PRO:O	3:O:174:ALA:HB2	2.00	0.61
2:M:76:VAL:O	2:M:77:GLU:CB	2.47	0.61
1:I:25:TYR:CB	2:L:64:THR:O	2.49	0.61
4:H:84:HIS:C	4:H:86:VAL:N	2.53	0.61
1:A:11:GLY:HA3	2:F:50:VAL:CA	2.31	0.61
3:G:170:PRO:O	3:G:174:ALA:HB2	2.00	0.61
3:G:135:GLU:O	3:G:137:LEU:N	2.33	0.60
1:B:10:ALA:H	2:D:50:VAL:CA	2.14	0.60
1:C:44:GLY:HA2	2:F:69:ALA:HB2	1.77	0.60
1:C:12:PRO:N	2:E:49:GLU:CB	2.64	0.60
1:I:25:TYR:O	2:L:65:GLY:CA	2.49	0.60
4:P:84:HIS:O	4:P:86:VAL:CA	2.48	0.60
3:O:158:THR:C	3:O:161:VAL:CB	2.70	0.60
3:G:158:THR:C	3:G:161:VAL:CB	2.70	0.60
1:C:12:PRO:O	1:C:13:ALA:HB3	2.02	0.60
2:D:359:SER:C	2:D:361:LEU:H	2.04	0.60
1:I:12:PRO:O	1:I:13:ALA:HB3	2.01	0.60
3:G:160:ARG:O	3:G:164:LEU:CB	2.50	0.60
1:A:12:PRO:O	1:A:13:ALA:HB3	2.01	0.60
1:A:43:ASP:C	2:D:69:ALA:HB3	2.22	0.60
1:K:11:GLY:HA3	2:M:50:VAL:H	1.66	0.60
1:K:12:PRO:O	1:K:13:ALA:HB3	2.02	0.59
1:J:12:PRO:O	1:J:13:ALA:HB3	2.02	0.59
1:K:27:ILE:HA	1:K:71:LEU:H	1.68	0.59
1:I:241:LEU:O	1:I:245:SER:N	2.33	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:334:GLU:CB	2:D:361:LEU:CB	2.80	0.59
1:I:25:TYR:H	2:L:66:LEU:H	0.61	0.59
3:O:150:ILE:C	3:O:151:GLY:O	2.39	0.59
3:G:135:GLU:HA	3:G:138:ILE:N	2.17	0.59
1:I:56:SER:CB	2:N:30:GLY:CA	2.81	0.59
1:A:44:GLY:N	2:D:69:ALA:HB1	2.08	0.59
3:O:135:GLU:HA	3:O:138:ILE:N	2.17	0.59
1:B:12:PRO:O	1:B:13:ALA:HB3	2.01	0.59
3:O:135:GLU:O	3:O:137:LEU:N	2.33	0.59
1:K:70:PRO:CB	1:K:71:LEU:O	2.50	0.59
3:O:160:ARG:O	3:O:164:LEU:CB	2.50	0.59
1:J:263:THR:CB	2:L:125:ARG:CA	2.80	0.59
1:B:9:ILE:CB	2:D:52:GLU:N	2.66	0.59
1:I:292:SER:CB	2:N:292:ALA:CB	2.81	0.58
3:G:150:ILE:C	3:G:151:GLY:O	2.39	0.58
1:A:44:GLY:N	2:D:69:ALA:HB2	2.11	0.58
1:J:24:MET:HA	2:M:67:ASP:O	2.04	0.58
1:C:197:ARG:O	1:C:368:VAL:HA	2.04	0.58
1:I:208:GLY:O	1:I:507:CYS:O	2.21	0.58
2:L:134:GLY:HA2	2:L:430:ARG:O	2.04	0.58
3:G:47:MET:C	3:G:49:ALA:N	2.57	0.57
4:H:84:HIS:C	4:H:86:VAL:H	2.06	0.57
1:C:189:VAL:O	1:C:304:TYR:O	2.22	0.57
1:C:344:MET:CB	2:F:272:ALA:CB	2.81	0.57
1:A:267:VAL:CB	2:F:125:ARG:HA	2.34	0.57
1:I:11:GLY:N	2:N:50:VAL:O	2.38	0.57
3:O:186:ARG:O	3:O:190:ASP:CB	2.53	0.57
3:G:47:MET:C	3:G:49:ALA:H	2.08	0.57
1:J:241:LEU:O	1:J:245:SER:N	2.33	0.57
1:C:52:TYR:C	1:C:295:PRO:CB	2.69	0.57
1:C:420:PRO:N	1:C:496:GLN:HA	2.19	0.57
1:K:259:GLY:O	2:M:297:ARG:N	2.34	0.57
1:K:241:LEU:O	1:K:245:SER:N	2.32	0.56
3:G:135:GLU:C	3:G:137:LEU:H	2.03	0.56
1:I:419:PHE:HA	1:I:420:PRO:C	2.25	0.56
1:I:352:PRO:CB	2:L:269:GLU:O	2.53	0.56
1:C:241:LEU:O	1:C:245:SER:N	2.31	0.56
3:O:132:ARG:O	3:O:133:TYR:C	2.38	0.56
3:O:47:MET:C	3:O:49:ALA:H	2.09	0.56
3:O:48:GLU:O	3:O:51:LYS:N	2.38	0.56
1:I:25:TYR:N	2:L:65:GLY:HA2	2.19	0.56
2:M:334:GLU:O	2:M:360:ARG:N	2.37	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:G:186:ARG:O	3:G:190:ASP:CB	2.53	0.56
3:O:47:MET:C	3:O:49:ALA:N	2.57	0.56
1:J:263:THR:CB	2:L:125:ARG:O	2.53	0.56
1:A:241:LEU:O	1:A:245:SER:CB	2.54	0.56
1:I:25:TYR:CB	2:L:65:GLY:CA	2.79	0.56
1:C:419:PHE:HA	1:C:420:PRO:C	2.25	0.56
4:P:86:VAL:O	4:P:87:GLU:C	2.44	0.56
2:N:136:SER:CB	2:N:430:ARG:CB	2.84	0.56
3:G:189:GLU:CB	3:G:189:GLU:HA	2.18	0.56
3:G:137:LEU:O	3:G:140:VAL:CB	2.54	0.56
1:K:419:PHE:HA	1:K:420:PRO:C	2.25	0.56
1:B:419:PHE:HA	1:B:420:PRO:C	2.25	0.56
1:C:430:LEU:O	1:C:432:THR:N	2.38	0.56
3:O:45:GLU:C	3:O:47:MET:N	2.58	0.56
1:C:344:MET:CB	2:F:272:ALA:CA	2.84	0.56
3:G:132:ARG:N	3:G:134:ALA:CB	2.68	0.56
1:I:25:TYR:H	2:L:65:GLY:C	2.04	0.56
1:I:266:LEU:CB	2:N:124:ARG:CA	2.82	0.56
3:O:137:LEU:O	3:O:140:VAL:CB	2.54	0.55
3:O:158:THR:HA	3:O:161:VAL:CB	2.37	0.55
3:G:142:ASN:CB	3:G:142:ASN:HA	2.17	0.55
2:L:359:SER:CB	2:L:362:MET:H	2.18	0.55
3:O:142:ASN:HA	3:O:142:ASN:CB	2.16	0.55
3:G:132:ARG:O	3:G:133:TYR:C	2.37	0.55
1:J:419:PHE:HA	1:J:420:PRO:C	2.25	0.55
1:C:266:LEU:CB	2:E:124:ARG:CA	2.80	0.55
3:G:48:GLU:O	3:G:51:LYS:N	2.39	0.55
1:I:25:TYR:C	2:L:65:GLY:HA2	2.26	0.55
1:K:11:GLY:HA2	2:M:49:GLU:HA	1.88	0.55
3:G:44:ARG:C	3:G:47:MET:CB	2.72	0.55
1:K:10:ALA:O	2:M:50:VAL:N	2.39	0.55
1:A:419:PHE:HA	1:A:420:PRO:C	2.25	0.55
3:O:136:ALA:O	3:O:140:VAL:CB	2.55	0.54
3:O:137:LEU:O	3:O:140:VAL:N	2.40	0.54
4:P:77:LEU:O	4:P:78:LYS:O	2.23	0.54
1:B:241:LEU:O	1:B:245:SER:N	2.31	0.54
3:G:158:THR:HA	3:G:161:VAL:CB	2.37	0.54
1:I:56:SER:CB	2:N:30:GLY:H	2.20	0.54
1:K:189:VAL:CB	1:K:304:TYR:CB	2.85	0.54
1:A:25:TYR:H	2:D:66:LEU:H	1.56	0.54
3:G:137:LEU:O	3:G:140:VAL:N	2.40	0.54
1:A:71:LEU:CB	1:A:188:PRO:C	2.76	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:24:MET:CB	2:M:66:LEU:CA	2.80	0.54
3:G:136:ALA:O	3:G:140:VAL:CB	2.55	0.54
3:O:7:THR:O	3:O:9:MET:N	2.41	0.54
1:I:225:ALA:O	1:I:406:PHE:HA	2.07	0.54
1:K:225:ALA:O	1:K:406:PHE:HA	2.07	0.54
3:O:132:ARG:N	3:O:134:ALA:CB	2.68	0.53
3:G:167:VAL:C	3:G:169:ILE:N	2.61	0.53
2:E:153:PHE:CB	2:E:338:GLN:HA	2.38	0.53
1:A:292:SER:CB	2:F:292:ALA:CB	2.86	0.53
1:A:296:VAL:HA	1:A:333:ALA:HB1	1.90	0.53
1:C:225:ALA:O	1:C:406:PHE:HA	2.08	0.53
1:B:225:ALA:O	1:B:406:PHE:HA	2.08	0.53
1:A:225:ALA:O	1:A:406:PHE:HA	2.08	0.53
3:O:44:ARG:C	3:O:47:MET:CB	2.72	0.53
1:B:224:ALA:CA	1:B:405:ALA:HB3	2.37	0.53
1:K:224:ALA:CA	1:K:405:ALA:HB3	2.37	0.53
1:I:259:GLY:O	2:N:297:ARG:N	2.42	0.53
1:J:296:VAL:HA	1:J:333:ALA:HB1	1.90	0.53
1:J:227:PRO:HA	1:J:384:VAL:CB	2.39	0.53
3:G:138:ILE:O	3:G:139:ARG:O	2.27	0.53
1:K:44:GLY:CA	2:N:69:ALA:HB3	2.14	0.53
4:P:86:VAL:C	4:P:88:GLY:N	2.62	0.53
2:L:153:PHE:CB	2:L:338:GLN:HA	2.39	0.53
1:C:430:LEU:C	1:C:432:THR:H	2.12	0.53
1:B:296:VAL:HA	1:B:333:ALA:HB1	1.90	0.53
3:O:145:THR:O	3:O:149:LYS:CB	2.57	0.53
3:O:42:LEU:O	3:O:45:GLU:CB	2.57	0.53
2:F:426:GLY:O	1:K:125:PRO:CA	2.57	0.53
4:H:77:LEU:O	4:H:78:LYS:C	2.32	0.53
4:H:76:GLY:O	4:H:80:ALA:HB1	2.06	0.53
2:M:153:PHE:CB	2:M:338:GLN:HA	2.39	0.53
1:C:259:GLY:C	2:E:296:GLU:C	2.65	0.53
1:I:132:GLY:HA3	1:I:371:LEU:C	2.28	0.53
1:A:227:PRO:HA	1:A:384:VAL:CB	2.39	0.53
3:G:166:GLN:O	3:G:169:ILE:CB	2.57	0.53
2:D:153:PHE:CB	2:D:338:GLN:HA	2.39	0.53
3:O:138:ILE:O	3:O:139:ARG:O	2.27	0.53
1:I:43:ASP:HA	2:L:69:ALA:HB2	1.88	0.53
1:A:224:ALA:CA	1:A:405:ALA:HB3	2.37	0.53
1:I:260:ASN:N	2:N:296:GLU:HA	2.23	0.53
2:F:153:PHE:CB	2:F:338:GLN:HA	2.39	0.53
2:N:153:PHE:CB	2:N:338:GLN:HA	2.39	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:419:PHE:C	1:A:497:GLN:O	2.47	0.53
1:I:227:PRO:HA	1:I:384:VAL:CB	2.39	0.53
1:C:296:VAL:HA	1:C:333:ALA:HB1	1.91	0.53
3:G:39:PHE:O	3:G:42:LEU:CB	2.57	0.53
1:A:419:PHE:CB	1:A:497:GLN:O	2.56	0.53
3:G:145:THR:O	3:G:149:LYS:CB	2.57	0.52
1:C:227:PRO:HA	1:C:384:VAL:CB	2.39	0.52
1:B:227:PRO:HA	1:B:384:VAL:CB	2.39	0.52
1:C:266:LEU:C	2:E:124:ARG:HA	2.30	0.52
3:G:45:GLU:C	3:G:47:MET:N	2.58	0.52
1:I:189:VAL:HA	1:I:308:THR:CB	2.39	0.52
1:A:81:ASN:HA	1:A:282:MET:O	2.10	0.52
1:I:296:VAL:HA	1:I:333:ALA:HB1	1.91	0.52
3:G:141:ALA:CA	3:G:145:THR:H	2.22	0.52
1:J:225:ALA:O	1:J:406:PHE:HA	2.08	0.52
3:O:173:ARG:O	3:O:177:ARG:CB	2.58	0.52
3:G:165:GLU:O	3:G:166:GLN:C	2.47	0.52
2:N:334:GLU:O	2:N:360:ARG:N	2.43	0.52
1:K:227:PRO:HA	1:K:384:VAL:CB	2.39	0.52
3:G:138:ILE:C	3:G:139:ARG:O	2.45	0.52
3:O:166:GLN:O	3:O:169:ILE:CB	2.57	0.52
2:L:359:SER:CA	2:L:362:MET:H	2.23	0.52
1:J:69:LEU:C	1:J:70:PRO:O	2.47	0.52
3:G:42:LEU:O	3:G:45:GLU:CB	2.57	0.52
1:I:44:GLY:N	2:L:69:ALA:HB2	1.76	0.52
3:O:167:VAL:C	3:O:169:ILE:N	2.61	0.52
1:A:52:TYR:O	1:A:53:GLU:CB	2.58	0.52
1:C:52:TYR:O	1:C:53:GLU:CB	2.58	0.52
1:K:11:GLY:HA3	2:M:49:GLU:HA	1.90	0.52
1:I:259:GLY:O	2:N:298:ALA:N	2.43	0.52
1:I:52:TYR:O	1:I:53:GLU:CB	2.58	0.52
1:K:52:TYR:O	1:K:53:GLU:CB	2.58	0.51
1:I:224:ALA:CA	1:I:405:ALA:HB3	2.37	0.51
3:O:205:GLU:CB	3:O:205:GLU:N	2.67	0.51
3:O:165:GLU:O	3:O:166:GLN:C	2.47	0.51
1:B:224:ALA:HB2	1:B:405:ALA:CB	2.31	0.51
1:K:296:VAL:HA	1:K:333:ALA:HB1	1.90	0.51
1:I:204:PRO:CB	1:I:435:LEU:CB	2.89	0.51
1:B:52:TYR:O	1:B:53:GLU:CB	2.58	0.51
3:O:141:ALA:CA	3:O:145:THR:H	2.22	0.51
3:G:52:ALA:CB	3:G:52:ALA:C	2.74	0.51
3:G:7:THR:O	3:G:9:MET:N	2.42	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:202:ASN:HA	1:C:434:ALA:O	2.11	0.51
3:G:171:GLY:O	3:G:174:ALA:HB3	2.11	0.51
3:G:173:ARG:O	3:G:177:ARG:CB	2.58	0.51
3:O:171:GLY:O	3:O:174:ALA:HB3	2.11	0.51
3:O:138:ILE:C	3:O:139:ARG:O	2.45	0.51
3:O:52:ALA:CB	3:O:52:ALA:C	2.74	0.51
1:I:266:LEU:CB	2:N:124:ARG:HA	2.41	0.51
3:G:183:LEU:O	3:G:186:ARG:CB	2.59	0.51
1:J:71:LEU:O	1:J:188:PRO:HA	2.10	0.50
3:O:183:LEU:O	3:O:186:ARG:CB	2.60	0.50
1:A:69:LEU:O	1:A:71:LEU:O	2.29	0.50
4:P:84:HIS:O	4:P:85:ASP:C	2.47	0.50
1:A:43:ASP:O	2:D:69:ALA:HB3	2.12	0.50
1:C:73:VAL:O	1:C:186:THR:HA	2.12	0.50
3:G:194:LEU:CB	3:G:194:LEU:C	2.73	0.50
3:O:132:ARG:C	3:O:134:ALA:H	2.13	0.50
1:K:11:GLY:HA3	2:M:50:VAL:N	2.27	0.50
1:J:52:TYR:O	1:J:53:GLU:CB	2.58	0.50
3:O:148:LYS:O	3:O:152:GLU:CA	2.59	0.50
1:A:266:LEU:CB	2:F:124:ARG:CA	2.89	0.50
1:A:73:VAL:O	1:A:186:THR:HA	2.12	0.50
3:G:146:ARG:O	3:G:147:LEU:C	2.50	0.50
1:J:224:ALA:CA	1:J:405:ALA:HB3	2.37	0.50
2:F:426:GLY:C	1:K:125:PRO:O	2.48	0.50
1:K:216:PHE:HA	1:K:429:SER:CB	2.42	0.50
3:G:132:ARG:C	3:G:134:ALA:H	2.13	0.49
2:N:149:LYS:O	2:N:333:THR:CB	2.59	0.49
2:L:150:LEU:CB	2:L:335:GLY:O	2.60	0.49
1:B:73:VAL:O	1:B:186:THR:HA	2.12	0.49
3:O:142:ASN:CB	3:O:142:ASN:N	2.67	0.49
1:C:352:PRO:O	2:F:269:GLU:CB	2.60	0.49
1:J:224:ALA:HB2	1:J:405:ALA:CB	2.31	0.49
1:K:73:VAL:O	1:K:186:THR:HA	2.12	0.49
1:J:73:VAL:O	1:J:186:THR:HA	2.11	0.49
3:G:205:GLU:N	3:G:205:GLU:CB	2.66	0.49
3:O:43:VAL:O	3:O:44:ARG:C	2.51	0.49
1:A:11:GLY:CA	2:F:50:VAL:N	2.73	0.49
1:J:9:ILE:CA	2:L:50:VAL:O	2.57	0.49
2:F:149:LYS:O	2:F:333:THR:CB	2.59	0.49
2:E:149:LYS:O	2:E:333:THR:CB	2.59	0.49
3:O:146:ARG:O	3:O:149:LYS:N	2.45	0.49
2:D:149:LYS:O	2:D:333:THR:CB	2.59	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:G:148:LYS:O	3:G:152:GLU:CA	2.59	0.49
3:G:146:ARG:O	3:G:149:LYS:N	2.45	0.49
1:C:344:MET:CB	2:F:272:ALA:HA	2.42	0.49
3:O:49:ALA:O	3:O:52:ALA:CB	2.53	0.49
3:O:7:THR:O	3:O:8:ARG:O	2.30	0.49
2:N:61:GLU:HA	2:N:229:ILE:CB	2.42	0.49
1:K:557:GLU:C	1:K:559:PHE:N	2.66	0.49
2:E:150:LEU:CB	2:E:335:GLY:O	2.61	0.49
1:A:557:GLU:C	1:A:559:PHE:N	2.66	0.49
1:J:557:GLU:C	1:J:559:PHE:N	2.66	0.49
1:J:9:ILE:HA	2:L:50:VAL:CB	2.42	0.49
2:N:150:LEU:CB	2:N:335:GLY:O	2.61	0.49
2:M:150:LEU:CB	2:M:335:GLY:O	2.61	0.49
3:G:43:VAL:O	3:G:44:ARG:C	2.51	0.49
2:L:149:LYS:O	2:L:333:THR:CB	2.59	0.49
3:O:198:LYS:O	3:O:199:GLY:O	2.31	0.49
2:D:150:LEU:CB	2:D:335:GLY:O	2.60	0.49
1:A:259:GLY:H	2:F:296:GLU:HA	1.68	0.49
3:O:146:ARG:O	3:O:147:LEU:C	2.50	0.49
4:H:84:HIS:O	4:H:85:ASP:C	2.43	0.49
2:M:149:LYS:O	2:M:333:THR:CB	2.60	0.49
3:O:134:ALA:O	3:O:137:LEU:CB	2.61	0.48
1:I:24:MET:CB	2:L:66:LEU:N	2.76	0.48
3:G:198:LYS:O	3:G:199:GLY:O	2.31	0.48
1:B:557:GLU:C	1:B:559:PHE:N	2.66	0.48
1:I:73:VAL:O	1:I:186:THR:HA	2.12	0.48
3:O:3:GLN:O	3:O:6:PRO:N	2.46	0.48
1:K:260:ASN:N	2:M:296:GLU:HA	1.95	0.48
3:O:198:LYS:O	3:O:199:GLY:C	2.52	0.48
1:I:557:GLU:C	1:I:559:PHE:N	2.66	0.48
3:G:134:ALA:O	3:G:137:LEU:CB	2.62	0.48
3:G:3:GLN:O	3:G:6:PRO:N	2.47	0.48
1:C:224:ALA:CA	1:C:405:ALA:HB3	2.37	0.48
1:C:44:GLY:HA2	2:F:69:ALA:HB3	1.84	0.48
3:O:200:LYS:HA	3:O:203:ALA:HB3	1.96	0.48
1:I:440:ARG:HA	1:I:444:ALA:O	2.14	0.48
1:J:440:ARG:HA	1:J:444:ALA:O	2.14	0.48
3:O:138:ILE:O	3:O:142:ASN:CB	2.62	0.48
3:O:48:GLU:CB	3:O:51:LYS:CB	2.92	0.48
1:C:189:VAL:HA	1:C:308:THR:CB	2.43	0.48
1:C:557:GLU:C	1:C:559:PHE:N	2.66	0.48
2:F:150:LEU:CB	2:F:335:GLY:O	2.61	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:G:135:GLU:HA	3:G:138:ILE:H	1.79	0.48
3:G:198:LYS:O	3:G:199:GLY:C	2.52	0.48
3:G:4:VAL:CA	3:G:5:SER:N	2.68	0.47
3:O:153:GLU:O	3:O:154:ILE:O	2.32	0.47
1:B:11:GLY:HA2	2:D:48:ILE:O	2.14	0.47
3:G:153:GLU:O	3:G:154:ILE:O	2.32	0.47
3:G:167:VAL:C	3:G:169:ILE:H	2.18	0.47
3:O:167:VAL:C	3:O:169:ILE:H	2.18	0.47
1:A:440:ARG:HA	1:A:444:ALA:O	2.14	0.47
4:P:65:GLY:CA	4:P:66:ARG:CB	2.93	0.47
3:G:48:GLU:CB	3:G:51:LYS:CB	2.92	0.47
1:C:24:MET:CA	2:F:66:LEU:HA	2.31	0.47
1:K:44:GLY:HA3	2:N:69:ALA:CB	2.40	0.47
3:G:138:ILE:O	3:G:142:ASN:CB	2.62	0.47
1:K:267:VAL:N	2:M:124:ARG:CB	2.78	0.47
1:K:440:ARG:HA	1:K:444:ALA:O	2.14	0.47
2:F:150:LEU:C	2:F:335:GLY:O	2.53	0.47
2:E:150:LEU:C	2:E:335:GLY:O	2.53	0.47
2:M:150:LEU:C	2:M:335:GLY:O	2.53	0.47
3:O:135:GLU:HA	3:O:138:ILE:H	1.80	0.47
3:G:200:LYS:HA	3:G:203:ALA:HB3	1.96	0.47
2:L:150:LEU:C	2:L:335:GLY:O	2.52	0.47
1:C:440:ARG:HA	1:C:444:ALA:O	2.14	0.47
1:B:9:ILE:CA	2:D:50:VAL:O	2.53	0.46
2:D:150:LEU:C	2:D:335:GLY:O	2.53	0.46
1:B:440:ARG:HA	1:B:444:ALA:O	2.14	0.46
3:O:200:LYS:CA	3:O:203:ALA:HB3	2.45	0.46
1:K:11:GLY:CA	2:M:49:GLU:CB	2.93	0.46
1:C:189:VAL:CB	1:C:305:VAL:N	2.78	0.46
1:J:419:PHE:O	1:J:496:GLN:CB	2.63	0.46
1:J:86:GLY:HA2	1:J:302:SER:CB	2.46	0.46
3:G:49:ALA:O	3:G:52:ALA:CB	2.53	0.46
1:B:475:ALA:O	4:H:102:ILE:CB	2.63	0.46
2:M:134:GLY:O	2:M:429:ASN:HA	2.14	0.46
1:I:71:LEU:CB	1:I:72:ALA:CA	2.92	0.46
2:N:150:LEU:C	2:N:335:GLY:O	2.53	0.46
2:D:359:SER:CB	2:D:362:MET:H	2.28	0.46
1:C:25:TYR:CA	2:F:65:GLY:HA2	2.36	0.46
1:A:224:ALA:HB2	1:A:405:ALA:CB	2.31	0.46
3:G:200:LYS:CA	3:G:203:ALA:HB3	2.45	0.46
3:O:194:LEU:C	3:O:194:LEU:CB	2.73	0.46
3:G:7:THR:O	3:G:8:ARG:O	2.30	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:G:40:PHE:O	3:G:43:VAL:N	2.49	0.45
3:G:138:ILE:CB	4:H:16:ALA:CB	2.94	0.45
1:I:352:PRO:CB	2:L:272:ALA:HB3	2.47	0.45
2:L:334:GLU:CA	2:L:361:LEU:CB	2.94	0.45
1:I:11:GLY:HA3	2:N:50:VAL:CB	2.38	0.45
3:O:52:ALA:O	3:O:55:GLN:O	2.34	0.45
1:I:475:ALA:HB1	2:L:398:ILE:O	2.16	0.45
1:I:44:GLY:N	2:L:69:ALA:HB3	1.77	0.45
1:K:70:PRO:N	1:K:72:ALA:HB2	2.32	0.45
1:I:241:LEU:O	1:I:245:SER:CB	2.64	0.45
3:G:35:LEU:O	3:G:38:GLU:CB	2.65	0.45
3:O:35:LEU:O	3:O:38:GLU:CB	2.65	0.45
3:G:52:ALA:O	3:G:55:GLN:O	2.34	0.45
2:L:334:GLU:O	2:L:361:LEU:CA	2.63	0.45
1:C:266:LEU:CB	2:E:124:ARG:CB	2.94	0.45
1:J:241:LEU:O	1:J:245:SER:CB	2.64	0.45
1:K:241:LEU:O	1:K:245:SER:CB	2.64	0.45
3:G:151:GLY:O	3:G:152:GLU:O	2.35	0.45
1:C:268:GLU:CB	2:E:126:LYS:CB	2.94	0.45
1:I:132:GLY:HA3	1:I:371:LEU:O	2.17	0.45
1:K:296:VAL:CA	1:K:333:ALA:HB1	2.47	0.45
3:O:4:VAL:CA	3:O:5:SER:N	2.68	0.45
3:G:179:ILE:O	3:G:180:GLN:C	2.56	0.45
1:K:189:VAL:C	1:K:304:TYR:CB	2.85	0.45
3:O:179:ILE:O	3:O:180:GLN:C	2.55	0.45
1:A:352:PRO:CB	2:D:269:GLU:O	2.64	0.45
1:C:131:GLY:O	1:C:371:LEU:CB	2.65	0.45
3:G:189:GLU:CB	3:G:189:GLU:N	2.69	0.44
3:G:142:ASN:N	3:G:142:ASN:CB	2.67	0.44
1:A:11:GLY:HA3	2:F:50:VAL:N	2.32	0.44
1:C:296:VAL:CA	1:C:333:ALA:HB1	2.47	0.44
3:G:141:ALA:HB1	3:G:145:THR:CB	2.47	0.44
1:K:259:GLY:H	2:M:296:GLU:CB	2.20	0.44
1:J:296:VAL:CA	1:J:333:ALA:HB1	2.47	0.44
3:O:141:ALA:HB1	3:O:145:THR:CB	2.47	0.44
2:D:153:PHE:O	2:D:338:GLN:HA	2.17	0.44
1:C:81:ASN:N	1:C:282:MET:O	2.46	0.44
1:C:314:ARG:HA	1:C:318:PHE:O	2.18	0.44
3:G:45:GLU:O	3:G:47:MET:N	2.50	0.44
1:B:296:VAL:CA	1:B:333:ALA:HB1	2.47	0.44
1:J:314:ARG:HA	1:J:318:PHE:O	2.17	0.44
1:K:11:GLY:CA	2:M:49:GLU:CA	2.92	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:G:175:GLN:O	3:G:177:ARG:N	2.51	0.44
3:O:175:GLN:O	3:O:177:ARG:N	2.51	0.44
1:A:296:VAL:CA	1:A:333:ALA:HB1	2.47	0.44
3:O:151:GLY:O	3:O:152:GLU:O	2.35	0.44
1:A:314:ARG:HA	1:A:318:PHE:O	2.18	0.44
1:B:314:ARG:HA	1:B:318:PHE:O	2.18	0.44
3:O:45:GLU:O	3:O:47:MET:N	2.50	0.44
2:E:153:PHE:O	2:E:338:GLN:HA	2.18	0.44
1:I:296:VAL:CA	1:I:333:ALA:HB1	2.47	0.44
1:K:314:ARG:HA	1:K:318:PHE:O	2.18	0.44
3:O:167:VAL:C	3:O:167:VAL:HA	2.16	0.44
1:B:9:ILE:C	2:D:50:VAL:CB	2.86	0.44
2:L:153:PHE:O	2:L:338:GLN:HA	2.18	0.44
2:N:349:TYR:HA	2:N:350:PRO:C	2.38	0.43
1:A:71:LEU:CA	1:A:189:VAL:H	2.27	0.43
1:A:44:GLY:N	2:D:69:ALA:HB3	2.12	0.43
4:P:86:VAL:C	4:P:88:GLY:H	2.19	0.43
2:N:153:PHE:O	2:N:338:GLN:HA	2.18	0.43
1:I:314:ARG:HA	1:I:318:PHE:O	2.18	0.43
2:D:349:TYR:HA	2:D:350:PRO:C	2.38	0.43
1:B:471:VAL:CB	4:H:98:ILE:HA	2.48	0.43
1:K:224:ALA:HB2	1:K:405:ALA:CB	2.32	0.43
2:M:153:PHE:O	2:M:338:GLN:HA	2.18	0.43
1:K:208:GLY:O	1:K:507:CYS:O	2.35	0.43
1:K:69:LEU:CA	1:K:72:ALA:CB	2.97	0.43
1:I:69:LEU:CB	1:I:71:LEU:N	2.82	0.43
1:B:263:THR:CA	2:D:124:ARG:C	2.86	0.43
2:M:349:TYR:HA	2:M:350:PRO:C	2.39	0.43
1:J:75:LEU:O	1:J:184:TYR:HA	2.19	0.43
1:I:255:CYS:HA	1:I:290:ASN:CB	2.49	0.43
3:O:189:GLU:N	3:O:189:GLU:CB	2.69	0.43
3:O:4:VAL:C	3:O:6:PRO:N	2.71	0.43
2:F:258:THR:HA	2:F:259:ASP:HA	1.85	0.43
3:O:140:VAL:O	3:O:144:GLU:N	2.47	0.43
3:O:189:GLU:HA	3:O:189:GLU:CB	2.18	0.43
3:O:40:PHE:O	3:O:43:VAL:CB	2.67	0.43
1:K:75:LEU:O	1:K:184:TYR:HA	2.19	0.43
2:F:427:GLN:CB	1:K:126:GLY:HA2	2.46	0.43
1:B:241:LEU:O	1:B:245:SER:CB	2.67	0.43
2:E:258:THR:HA	2:E:259:ASP:HA	1.85	0.43
1:A:255:CYS:HA	1:A:290:ASN:CB	2.49	0.43
3:O:135:GLU:O	3:O:139:ARG:CB	2.67	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:G:135:GLU:O	3:G:139:ARG:CB	2.67	0.43
3:G:175:GLN:O	3:G:178:PHE:N	2.51	0.43
1:K:255:CYS:HA	1:K:290:ASN:CB	2.49	0.42
2:F:349:TYR:HA	2:F:350:PRO:C	2.39	0.42
1:K:52:TYR:C	1:K:295:PRO:CB	2.77	0.42
1:J:266:LEU:CB	2:L:124:ARG:CB	2.97	0.42
1:B:255:CYS:HA	1:B:290:ASN:CB	2.49	0.42
2:F:153:PHE:O	2:F:338:GLN:HA	2.18	0.42
3:O:174:ALA:O	3:O:175:GLN:O	2.37	0.42
1:C:241:LEU:O	1:C:245:SER:CB	2.67	0.42
1:B:75:LEU:O	1:B:184:TYR:HA	2.19	0.42
3:G:40:PHE:O	3:G:43:VAL:CB	2.67	0.42
1:I:25:TYR:O	2:L:65:GLY:HA3	2.16	0.42
1:I:346:ALA:HB2	2:L:272:ALA:HB2	2.01	0.42
2:D:189:VAL:O	2:D:217:SER:HA	2.19	0.42
2:L:349:TYR:HA	2:L:350:PRO:C	2.38	0.42
1:I:25:TYR:N	2:L:65:GLY:CA	2.82	0.42
2:E:189:VAL:O	2:E:217:SER:HA	2.20	0.42
2:L:189:VAL:O	2:L:217:SER:HA	2.20	0.42
1:J:255:CYS:HA	1:J:290:ASN:CB	2.49	0.42
1:C:75:LEU:O	1:C:184:TYR:HA	2.19	0.42
1:B:70:PRO:O	1:B:71:LEU:CB	2.68	0.42
1:K:69:LEU:CA	1:K:72:ALA:HB2	2.49	0.42
1:A:241:LEU:O	1:A:244:TRP:O	2.38	0.42
2:E:349:TYR:HA	2:E:350:PRO:C	2.39	0.42
1:I:75:LEU:O	1:I:184:TYR:HA	2.18	0.42
3:G:4:VAL:C	3:G:6:PRO:N	2.71	0.42
2:F:189:VAL:O	2:F:217:SER:HA	2.20	0.42
1:J:429:SER:C	1:J:431:PHE:H	2.23	0.42
1:A:133:MET:O	1:A:148:LEU:HA	2.20	0.42
1:C:430:LEU:C	1:C:432:THR:N	2.73	0.42
1:C:260:ASN:HA	2:E:296:GLU:O	2.20	0.41
3:O:175:GLN:O	3:O:178:PHE:N	2.51	0.41
1:J:133:MET:O	1:J:148:LEU:HA	2.20	0.41
1:A:221:GLY:O	1:A:366:GLY:HA2	2.21	0.41
3:O:48:GLU:O	3:O:51:LYS:CA	2.67	0.41
1:B:227:PRO:CB	1:B:384:VAL:CB	2.98	0.41
1:K:227:PRO:CB	1:K:384:VAL:CB	2.99	0.41
2:M:189:VAL:O	2:M:217:SER:HA	2.20	0.41
1:A:75:LEU:O	1:A:184:TYR:HA	2.19	0.41
3:O:134:ALA:O	4:P:16:ALA:HB2	2.19	0.41
1:C:202:ASN:O	1:C:435:LEU:HA	2.20	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:G:43:VAL:O	3:G:45:GLU:N	2.54	0.41
2:L:359:SER:O	2:L:361:LEU:N	2.53	0.41
1:C:25:TYR:N	2:F:66:LEU:N	2.31	0.41
1:C:133:MET:O	1:C:148:LEU:HA	2.20	0.41
2:N:189:VAL:O	2:N:217:SER:HA	2.20	0.41
1:C:255:CYS:HA	1:C:290:ASN:CB	2.49	0.41
1:B:221:GLY:O	1:B:366:GLY:HA2	2.21	0.41
2:D:149:LYS:CB	2:D:333:THR:HA	2.51	0.41
1:K:133:MET:O	1:K:148:LEU:HA	2.21	0.41
1:B:133:MET:O	1:B:148:LEU:HA	2.20	0.41
2:F:149:LYS:CB	2:F:333:THR:HA	2.51	0.41
3:O:148:LYS:C	3:O:149:LYS:O	2.59	0.41
1:B:9:ILE:CB	2:D:51:SER:C	2.89	0.41
1:C:11:GLY:CA	2:E:50:VAL:N	2.57	0.41
1:B:141:PHE:O	1:B:143:PHE:O	2.39	0.41
1:A:56:SER:CB	2:F:30:GLY:H	2.34	0.41
1:I:133:MET:O	1:I:148:LEU:HA	2.21	0.41
1:K:221:GLY:O	1:K:366:GLY:HA2	2.21	0.41
1:K:141:PHE:O	1:K:143:PHE:O	2.39	0.41
3:O:43:VAL:O	3:O:45:GLU:N	2.54	0.41
2:N:149:LYS:CB	2:N:333:THR:HA	2.51	0.41
1:A:227:PRO:CB	1:A:384:VAL:CB	2.99	0.41
1:I:227:PRO:CB	1:I:384:VAL:CB	2.99	0.41
1:J:221:GLY:O	1:J:366:GLY:HA2	2.20	0.41
1:C:221:GLY:O	1:C:366:GLY:HA2	2.21	0.41
1:C:141:PHE:O	1:C:143:PHE:O	2.39	0.41
3:G:48:GLU:O	3:G:51:LYS:CA	2.68	0.41
3:G:146:ARG:O	3:G:149:LYS:CB	2.68	0.41
2:L:359:SER:CB	2:L:362:MET:N	2.83	0.41
1:C:81:ASN:HA	1:C:282:MET:O	2.21	0.41
1:J:208:GLY:O	1:J:507:CYS:N	2.53	0.41
3:G:174:ALA:O	3:G:175:GLN:O	2.36	0.40
1:C:227:PRO:CB	1:C:384:VAL:CB	2.99	0.40
1:I:221:GLY:O	1:I:366:GLY:HA2	2.21	0.40
3:O:146:ARG:O	3:O:149:LYS:CB	2.69	0.40
2:M:149:LYS:CB	2:M:333:THR:HA	2.51	0.40
1:A:226:ILE:O	1:A:384:VAL:N	2.55	0.40
1:I:226:ILE:O	1:I:384:VAL:N	2.55	0.40
4:P:94:VAL:O	4:P:95:ARG:C	2.58	0.40
3:G:148:LYS:C	3:G:149:LYS:O	2.60	0.40
1:I:24:MET:CB	2:L:66:LEU:CA	2.99	0.40
2:L:149:LYS:CB	2:L:333:THR:HA	2.51	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:27:ILE:HA	1:K:71:LEU:N	2.33	0.40
1:A:259:GLY:C	2:F:296:GLU:HA	2.41	0.40
2:N:258:THR:HA	2:N:259:ASP:HA	1.85	0.40
1:J:141:PHE:O	1:J:143:PHE:O	2.39	0.40
2:L:334:GLU:O	2:L:360:ARG:C	2.56	0.40
1:A:259:GLY:O	2:F:296:GLU:O	2.39	0.40
1:J:227:PRO:CB	1:J:384:VAL:CB	2.99	0.40
1:J:226:ILE:O	1:J:384:VAL:N	2.55	0.40
1:C:226:ILE:O	1:C:384:VAL:N	2.55	0.40
1:I:141:PHE:O	1:I:143:PHE:O	2.39	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:6:ILE:CB	2:M:24:ALA:O[5_555]	1.43	0.77
1:J:1:MET:N	2:M:9:THR:CA[5_555]	1.83	0.37
1:J:5:VAL:CA	2:M:24:ALA:CB[5_555]	1.92	0.28

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	557/578 (96%)	488 (88%)	52 (9%)	17 (3%)	7	57
1	B	557/578 (96%)	493 (88%)	48 (9%)	16 (3%)	7	58
1	C	557/578 (96%)	491 (88%)	48 (9%)	18 (3%)	6	56
1	I	557/578 (96%)	491 (88%)	50 (9%)	16 (3%)	7	58
1	J	557/578 (96%)	492 (88%)	48 (9%)	17 (3%)	7	57
1	K	557/578 (96%)	493 (88%)	47 (8%)	17 (3%)	7	57
2	D	446/478 (93%)	420 (94%)	17 (4%)	9 (2%)	11	67
2	E	446/478 (93%)	421 (94%)	16 (4%)	9 (2%)	11	67
2	F	446/478 (93%)	421 (94%)	16 (4%)	9 (2%)	11	67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	L	446/478 (93%)	419 (94%)	17 (4%)	10 (2%)	10	64
2	M	446/478 (93%)	422 (95%)	15 (3%)	9 (2%)	11	67
2	N	446/478 (93%)	422 (95%)	15 (3%)	9 (2%)	11	67
3	G	125/223 (56%)	76 (61%)	20 (16%)	29 (23%)	0	3
3	O	125/223 (56%)	76 (61%)	20 (16%)	29 (23%)	0	3
4	H	102/104 (98%)	87 (85%)	9 (9%)	6 (6%)	2	38
4	P	102/104 (98%)	86 (84%)	11 (11%)	5 (5%)	3	43
All	All	6472/6990 (93%)	5798 (90%)	449 (7%)	225 (4%)	6	54

All (225) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	PRO
1	A	19	MET
1	A	53	GLU
1	A	143	PHE
1	A	227	PRO
1	A	256	GLY
1	A	260	ASN
1	A	325	ASP
1	A	394	PRO
1	A	395	VAL
1	A	558	GLU
1	B	12	PRO
1	B	19	MET
1	B	53	GLU
1	B	143	PHE
1	B	227	PRO
1	B	256	GLY
1	B	260	ASN
1	B	325	ASP
1	B	394	PRO
1	B	395	VAL
1	B	558	GLU
1	C	12	PRO
1	C	19	MET
1	C	53	GLU
1	C	143	PHE
1	C	227	PRO
1	C	256	GLY

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Mol	Chain	Res	Type
1	C	260	ASN
1	C	325	ASP
1	C	394	PRO
1	C	395	VAL
1	C	431	PHE
1	C	558	GLU
2	D	52	GLU
2	D	79	VAL
2	D	316	MET
2	D	356	PRO
2	D	427	GLN
2	E	52	GLU
2	E	79	VAL
2	E	316	MET
2	E	356	PRO
2	E	427	GLN
2	F	52	GLU
2	F	316	MET
2	F	356	PRO
2	F	427	GLN
3	G	3	GLN
3	G	4	VAL
3	G	43	VAL
3	G	47	MET
3	G	48	GLU
3	G	140	VAL
3	G	149	LYS
3	G	152	GLU
3	G	161	VAL
3	G	172	ILE
3	G	174	ALA
4	H	63	MET
4	H	66	ARG
4	H	75	ALA
4	H	85	ASP
4	H	100	PHE
1	I	12	PRO
1	I	19	MET
1	I	53	GLU
1	I	143	PHE
1	I	227	PRO
1	I	256	GLY

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Mol	Chain	Res	Type
1	I	260	ASN
1	I	325	ASP
1	I	394	PRO
1	I	395	VAL
1	I	558	GLU
1	J	12	PRO
1	J	19	MET
1	J	53	GLU
1	J	143	PHE
1	J	227	PRO
1	J	256	GLY
1	J	260	ASN
1	J	325	ASP
1	J	394	PRO
1	J	395	VAL
1	J	430	LEU
1	J	558	GLU
1	K	12	PRO
1	K	19	MET
1	K	53	GLU
1	K	143	PHE
1	K	227	PRO
1	K	256	GLY
1	K	260	ASN
1	K	325	ASP
1	K	394	PRO
1	K	395	VAL
1	K	558	GLU
2	L	52	GLU
2	L	79	VAL
2	L	81	ARG
2	L	316	MET
2	L	356	PRO
2	L	427	GLN
2	M	52	GLU
2	M	316	MET
2	M	356	PRO
2	M	427	GLN
2	N	52	GLU
2	N	316	MET
2	N	356	PRO
2	N	427	GLN

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Mol	Chain	Res	Type
3	O	3	GLN
3	O	4	VAL
3	O	43	VAL
3	O	47	MET
3	O	48	GLU
3	O	140	VAL
3	O	149	LYS
3	O	152	GLU
3	O	161	VAL
3	O	172	ILE
3	O	174	ALA
3	O	200	LYS
4	P	63	MET
4	P	86	VAL
4	P	87	GLU
4	P	100	PHE
1	A	88	GLN
1	A	255	CYS
1	B	88	GLN
1	B	255	CYS
1	C	88	GLN
1	C	199	LEU
1	C	255	CYS
2	D	26	ASP
2	D	428	GLN
2	E	26	ASP
2	E	428	GLN
2	F	26	ASP
2	F	428	GLN
3	G	2	SER
3	G	6	PRO
3	G	150	ILE
3	G	151	GLY
3	G	185	GLN
3	G	200	LYS
4	H	64	ARG
1	I	88	GLN
1	I	255	CYS
1	J	88	GLN
1	J	255	CYS
1	K	71	LEU
1	K	88	GLN

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Mol	Chain	Res	Type
1	K	255	CYS
2	L	26	ASP
2	L	428	GLN
2	M	26	ASP
2	M	79	VAL
2	M	428	GLN
2	N	26	ASP
2	N	428	GLN
3	O	2	SER
3	O	6	PRO
3	O	13	GLN
3	O	150	ILE
3	O	151	GLY
3	O	185	GLN
1	A	109	HIS
1	B	109	HIS
1	C	109	HIS
3	G	13	GLN
3	G	139	ARG
3	G	155	LYS
3	G	162	ASN
3	G	165	GLU
1	I	109	HIS
1	J	109	HIS
1	K	109	HIS
3	O	139	ARG
3	O	155	LYS
3	O	162	ASN
3	O	165	GLU
1	A	71	LEU
3	G	45	GLU
3	G	186	ARG
2	N	79	VAL
3	O	45	GLU
3	O	137	LEU
3	O	186	ARG
4	P	85	ASP
1	A	374	GLU
1	B	374	GLU
1	C	374	GLU
2	D	317	PRO
2	E	317	PRO

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Mol	Chain	Res	Type
2	F	317	PRO
3	G	53	LEU
3	G	137	LEU
3	G	197	ILE
1	I	374	GLU
1	J	374	GLU
1	K	374	GLU
2	L	317	PRO
2	M	317	PRO
2	N	317	PRO
3	O	53	LEU
2	F	79	VAL
3	O	197	ILE
2	D	355	LEU
2	E	355	LEU
2	F	355	LEU
2	L	355	LEU
2	M	355	LEU
2	N	355	LEU
1	A	388	GLY
1	B	388	GLY
1	C	388	GLY
3	G	179	ILE
1	I	388	GLY
1	J	388	GLY
1	K	388	GLY
3	O	179	ILE
3	G	168	VAL
3	O	168	VAL

5.3.2 Protein sidechains ⓘ

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95th 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 ²)	Q<0.9
1	A	561/578 (97%)	1.37	116 (20%) 1 4	168, 196, 399, 399	0
1	B	561/578 (97%)	0.49	51 (9%) 9 15	97, 98, 159, 159	0
1	C	561/578 (97%)	1.01	99 (17%) 2 5	208, 224, 414, 414	0
1	I	561/578 (97%)	1.73	168 (29%) 1 3	198, 211, 393, 393	0
1	J	561/578 (97%)	0.41	40 (7%) 16 19	90, 94, 161, 161	0
1	K	561/578 (97%)	1.18	113 (20%) 2 4	207, 219, 403, 403	0
2	D	450/478 (94%)	0.72	59 (13%) 4 8	138, 159, 262, 262	0
2	E	450/478 (94%)	0.82	61 (13%) 4 8	157, 157, 176, 176	0
2	F	450/478 (94%)	0.87	75 (16%) 2 5	155, 241, 275, 275	0
2	L	450/478 (94%)	0.78	58 (12%) 4 9	145, 154, 244, 244	0
2	M	450/478 (94%)	0.81	61 (13%) 4 8	151, 151, 191, 191	0
2	N	450/478 (94%)	1.52	121 (26%) 1 4	181, 256, 256, 256	0
3	G	129/223 (57%)	-0.09	2 (1%) 68 56	71, 85, 85, 85	0
3	O	129/223 (57%)	0.04	1 (0%) 83 71	89, 89, 105, 105	0
4	H	104/104 (100%)	0.51	13 (12%) 5 9	159, 185, 185, 185	0
4	P	104/104 (100%)	0.44	9 (8%) 10 16	159, 167, 167, 167	0
All	All	6532/6990 (93%)	0.93	1047 (16%) 3 6	71, 176, 399, 414	0

All (1047) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	147	ILE	27.4
1	A	165	GLU	18.8
1	A	163	ALA	18.4
1	A	166	TYR	18.2
1	A	162	PRO	17.1

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Mol	Chain	Res	Type	RSRZ
1	I	164	GLY	16.1
2	N	192	ALA	15.5
1	I	146	LYS	15.4
1	I	180	GLU	14.4
1	A	128	GLU	13.6
2	N	191	PHE	13.5
1	I	134	VAL	13.5
1	A	155	GLY	12.8
2	N	193	ALA	12.8
1	I	181	LEU	12.7
1	I	139	PRO	12.7
1	A	164	GLY	12.4
1	I	145	HIS	12.1
1	C	77	PRO	12.1
1	K	77	PRO	11.6
1	A	118	ALA	11.4
1	I	77	PRO	11.4
1	A	181	LEU	11.3
1	K	78	GLY	11.2
2	N	218	VAL	11.1
1	I	140	GLU	11.0
1	A	117	TRP	11.0
1	I	78	GLY	10.7
1	C	183	MET	10.5
1	A	167	THR	10.5
2	M	121	PRO	10.5
1	I	138	VAL	10.4
1	I	118	ALA	10.3
1	C	165	GLU	10.2
2	N	80	ALA	10.2
1	A	119	TRP	10.1
1	A	173	VAL	10.1
1	I	119	TRP	10.0
2	M	302	GLU	10.0
1	A	147	ILE	9.6
1	C	47	ALA	9.6
1	A	135	LEU	9.5
1	C	166	TYR	9.5
1	A	146	LYS	9.5
2	N	81	ARG	9.4
1	I	135	LEU	9.3
1	A	77	PRO	9.3

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Mol	Chain	Res	Type	RSRZ
1	I	137	THR	9.2
1	I	136	GLY	9.1
1	A	129	VAL	9.1
2	N	190	VAL	9.1
2	L	77	GLU	9.0
2	M	300	VAL	9.0
1	A	170	GLU	8.8
2	N	83	GLY	8.8
1	C	169	GLU	8.7
1	K	576	ALA	8.7
2	E	150	LEU	8.7
1	A	134	VAL	8.7
2	N	66	LEU	8.7
1	C	171	PRO	8.7
2	N	358	LEU	8.6
1	I	76	GLY	8.6
1	C	170	GLU	8.6
1	A	182	LYS	8.4
1	K	82	GLY	8.4
1	K	345	PRO	8.4
2	M	301	VAL	8.3
2	D	28	ALA	8.1
1	C	182	LYS	8.1
2	M	122	VAL	8.0
2	D	27	LEU	8.0
1	A	116	LYS	7.9
1	A	136	GLY	7.9
1	A	145	HIS	7.9
2	N	76	VAL	7.9
2	D	121	PRO	7.9
2	N	121	PRO	7.8
1	C	29	LYS	7.7
2	L	20	PHE	7.7
2	N	82	LEU	7.7
1	A	156	ARG	7.7
1	I	371	LEU	7.6
2	L	122	VAL	7.6
4	H	76	GLY	7.6
1	K	323	MET	7.6
1	C	37	GLY	7.5
2	E	119	LEU	7.5
2	N	118	PRO	7.5

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Mol	Chain	Res	Type	RSRZ
1	A	183	MET	7.5
2	L	121	PRO	7.5
2	F	122	VAL	7.4
1	A	121	PRO	7.4
1	I	133	MET	7.3
1	C	1	MET	7.2
2	E	120	ASN	7.2
1	K	79	MET	7.2
1	C	36	VAL	7.2
2	D	118	PRO	7.0
1	I	148	LEU	7.0
1	K	197	ARG	7.0
1	C	376	GLY	6.9
1	A	169	GLU	6.9
2	N	220	PHE	6.9
1	I	163	ALA	6.9
2	N	79	VAL	6.9
1	I	182	LYS	6.9
2	L	21	VAL	6.9
2	F	121	PRO	6.8
2	D	67	ASP	6.8
1	I	165	GLU	6.8
1	B	109	HIS	6.8
1	A	122	MET	6.7
1	K	575	LYS	6.7
2	N	75	LEU	6.7
1	I	179	THR	6.7
4	H	24	SER	6.7
1	C	28	CYS	6.6
4	P	75	ALA	6.6
2	M	299	GLY	6.6
2	F	11	ILE	6.5
2	D	102	GLY	6.5
2	N	359	SER	6.5
1	A	120	THR	6.4
2	M	362	MET	6.4
2	N	258	THR	6.3
2	E	121	PRO	6.3
1	I	372	GLY	6.3
2	E	463	TYR	6.2
4	P	85	ASP	6.2
1	K	295	PRO	6.2

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Mol	Chain	Res	Type	RSRZ
2	M	360	ARG	6.2
1	A	123	VAL	6.2
2	N	219	LEU	6.2
2	E	335	GLY	6.2
1	B	110	ALA	6.2
2	N	77	GLU	6.1
2	N	147	GLY	6.1
1	B	111	LEU	6.1
1	I	563	PHE	6.1
1	A	403	VAL	6.1
2	D	119	LEU	6.1
1	I	316	GLN	6.0
2	N	113	PRO	6.0
2	N	78	ASP	6.0
2	N	122	VAL	6.0
1	C	368	VAL	6.0
1	I	117	TRP	6.0
2	D	22	GLU	6.0
1	K	434	ALA	5.9
1	I	173	VAL	5.9
1	I	551	ALA	5.9
1	K	324	ALA	5.9
1	A	13	ALA	5.9
2	D	75	LEU	5.9
2	L	76	VAL	5.9
1	A	554	VAL	5.8
1	C	3	GLN	5.8
2	M	361	LEU	5.8
1	I	122	MET	5.8
1	I	116	LYS	5.8
1	A	219	ALA	5.7
1	A	137	THR	5.7
1	A	62	GLU	5.7
1	A	140	GLU	5.7
1	C	168	VAL	5.6
1	J	471	VAL	5.6
1	K	322	LEU	5.6
2	N	194	MET	5.6
1	K	346	ALA	5.6
1	A	223	THR	5.6
1	A	171	PRO	5.6
1	I	42	LEU	5.6

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Mol	Chain	Res	Type	RSRZ
1	K	196	GLN	5.6
2	L	29	TYR	5.5
2	E	300	VAL	5.5
2	N	168	ALA	5.5
2	E	362	MET	5.5
1	C	117	TRP	5.5
1	K	195	VAL	5.5
1	K	251	VAL	5.5
1	I	223	THR	5.5
1	K	297	ALA	5.5
1	K	201	PRO	5.4
1	C	86	GLY	5.4
1	K	198	LYS	5.4
2	L	75	LEU	5.4
2	F	298	ALA	5.4
2	F	123	ALA	5.4
1	A	200	ASP	5.3
1	C	197	ARG	5.3
1	I	562	TYR	5.3
2	N	140	VAL	5.3
1	I	183	MET	5.3
1	I	79	MET	5.3
1	I	224	ALA	5.3
1	A	201	PRO	5.3
2	N	84	VAL	5.3
1	A	78	GLY	5.3
2	D	120	ASN	5.3
2	D	122	VAL	5.2
1	B	112	ASP	5.2
1	K	538	GLU	5.2
2	E	172	THR	5.2
1	K	202	ASN	5.2
1	I	174	VAL	5.2
2	N	242	ALA	5.2
1	I	144	THR	5.2
2	N	123	ALA	5.2
1	C	379	THR	5.1
1	I	178	GLY	5.1
2	E	375	HIS	5.1
2	N	350	PRO	5.1
2	E	118	PRO	5.1
1	A	115	LYS	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	193	ARG	5.0
1	I	158	LYS	5.0
2	D	24	ALA	5.0
1	I	560	PRO	5.0
1	C	167	THR	5.0
1	A	218	VAL	5.0
1	C	4	GLY	5.0
2	M	168	ALA	5.0
1	I	177	ASP	4.9
2	E	173	VAL	4.9
2	D	23	ASN	4.9
2	F	28	ALA	4.9
1	A	174	VAL	4.9
2	F	299	GLY	4.9
1	A	61	GLY	4.9
1	C	116	LYS	4.9
2	N	221	LEU	4.8
1	I	557	GLU	4.8
2	F	302	GLU	4.8
1	I	559	PHE	4.8
1	K	117	TRP	4.8
1	A	345	PRO	4.8
1	K	76	GLY	4.8
1	C	140	GLU	4.8
1	C	78	GLY	4.8
1	I	1	MET	4.8
2	E	88	MET	4.8
2	N	189	VAL	4.7
2	D	131	ILE	4.7
1	I	141	PHE	4.7
2	N	148	GLN	4.7
1	A	180	GLU	4.7
1	I	132	GLY	4.7
1	I	159	GLU	4.7
2	F	155	GLY	4.7
1	K	321	ALA	4.7
2	L	56	VAL	4.6
2	N	428	GLN	4.6
1	J	23	ARG	4.6
2	N	298	ALA	4.6
1	A	57	GLY	4.6
2	F	365	GLY	4.6

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Mol	Chain	Res	Type	RSRZ
1	I	558	GLU	4.5
2	L	412	LEU	4.5
2	F	297	ARG	4.5
2	N	169	ARG	4.5
2	N	67	ASP	4.5
2	N	117	LEU	4.5
1	C	502	GLU	4.5
1	I	352	PRO	4.5
1	I	84	TYR	4.5
2	D	117	LEU	4.4
1	A	58	LEU	4.4
1	K	551	ALA	4.4
1	B	471	VAL	4.4
1	K	165	GLU	4.4
1	C	180	GLU	4.4
2	F	119	LEU	4.4
2	F	118	PRO	4.4
1	I	536	ILE	4.4
2	D	301	VAL	4.4
1	A	112	ASP	4.4
2	D	101	ASP	4.4
1	C	275	PRO	4.3
1	I	296	VAL	4.3
1	A	114	GLU	4.3
2	D	26	ASP	4.3
1	I	41	ARG	4.3
1	A	12	PRO	4.3
2	E	168	ALA	4.3
2	N	238	ALA	4.3
1	C	531	LYS	4.3
1	K	114	GLU	4.3
1	K	164	GLY	4.3
1	K	163	ALA	4.3
2	D	103	LEU	4.3
1	C	367	LYS	4.3
2	E	83	GLY	4.2
1	C	17	LYS	4.2
1	K	80	LEU	4.2
1	A	553	TYR	4.2
2	M	408	ASP	4.2
2	E	82	LEU	4.2
2	N	427	GLN	4.2

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Mol	Chain	Res	Type	RSRZ
1	J	2	ILE	4.2
1	C	369	ILE	4.2
2	F	347	GLY	4.2
1	C	345	PRO	4.2
2	M	310	GLN	4.1
2	E	122	VAL	4.1
2	E	86	LYS	4.1
2	N	334	GLU	4.1
1	I	155	GLY	4.1
1	J	22	ALA	4.1
2	F	17	PRO	4.1
2	L	411	TYR	4.1
4	P	104	LEU	4.1
1	A	138	VAL	4.1
1	B	114	GLU	4.1
2	N	360	ARG	4.1
1	B	551	ALA	4.1
1	I	471	VAL	4.1
1	K	181	LEU	4.1
2	D	68	LEU	4.1
1	J	559	PHE	4.1
1	K	539	ILE	4.1
2	F	300	VAL	4.1
1	I	111	LEU	4.1
2	L	19	LEU	4.0
2	F	301	VAL	4.0
2	L	52	GLU	4.0
1	C	577	LEU	4.0
2	L	401	GLU	4.0
1	B	518	MET	4.0
2	M	129	GLN	4.0
1	A	139	PRO	4.0
1	C	46	THR	4.0
1	I	63	PRO	4.0
2	L	80	ALA	4.0
2	M	80	ALA	4.0
1	I	564	GLU	4.0
1	C	112	ASP	4.0
2	F	21	VAL	3.9
1	K	220	MET	3.9
2	L	34	ASP	3.9
2	F	86	LYS	3.9

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Mol	Chain	Res	Type	RSRZ
1	I	370	THR	3.9
1	I	143	PHE	3.9
1	A	20	LEU	3.9
1	C	16	ALA	3.9
2	E	299	GLY	3.9
1	J	207	THR	3.9
2	N	146	ARG	3.9
1	I	472	GLY	3.9
1	K	573	ALA	3.9
1	A	144	THR	3.9
1	I	218	VAL	3.9
1	I	403	VAL	3.8
1	K	81	ASN	3.8
1	A	111	LEU	3.8
2	D	302	GLU	3.8
1	K	65	VAL	3.8
1	A	127	ASP	3.8
2	N	141	MET	3.8
2	N	241	VAL	3.8
1	I	154	ARG	3.8
2	M	175	PRO	3.8
2	E	149	LYS	3.8
2	M	127	PRO	3.8
2	N	114	ILE	3.8
1	A	6	ILE	3.8
2	M	70	THR	3.8
2	D	80	ALA	3.7
1	C	2	ILE	3.7
1	K	108	VAL	3.7
1	I	550	ARG	3.7
1	I	353	TYR	3.7
2	N	429	ASN	3.7
1	K	387	PRO	3.7
2	E	462	TYR	3.7
2	L	53	GLU	3.7
1	K	510	LYS	3.7
1	B	499	ALA	3.7
4	H	38	GLU	3.7
2	N	86	LYS	3.7
1	A	172	VAL	3.7
1	C	223	THR	3.7
1	K	376	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	I	424	TRP	3.7
1	I	12	PRO	3.7
1	C	74	GLU	3.7
4	P	78	LYS	3.7
1	K	47	ALA	3.7
1	J	345	PRO	3.7
2	F	401	GLU	3.7
1	I	373	GLY	3.7
1	A	422	ILE	3.7
2	L	123	ALA	3.7
1	I	566	ALA	3.7
2	N	297	ARG	3.7
2	N	164	ALA	3.6
1	K	252	TYR	3.6
2	E	85	SER	3.6
2	L	97	GLY	3.6
1	K	351	PRO	3.6
2	M	11	ILE	3.6
4	H	29	ALA	3.6
1	K	435	LEU	3.6
2	N	254	LEU	3.6
1	C	139	PRO	3.6
2	N	235	PRO	3.6
1	I	176	GLU	3.6
1	A	222	GLY	3.6
2	M	298	ALA	3.6
2	M	172	THR	3.6
2	N	198	GLN	3.6
1	B	478	ASP	3.6
1	I	402	ILE	3.6
1	C	276	LYS	3.6
1	A	154	ARG	3.5
2	M	404	LEU	3.5
2	E	374	ASP	3.5
2	L	413	GLN	3.5
2	M	359	SER	3.5
1	K	550	ARG	3.5
1	K	296	VAL	3.5
4	H	75	ALA	3.5
1	C	532	ARG	3.5
2	N	7	GLU	3.5
1	B	479	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
2	F	295	TYR	3.5
1	B	552	ARG	3.5
1	C	150	PRO	3.5
1	C	35	LEU	3.5
1	C	377	ALA	3.5
2	F	224	ALA	3.5
1	C	73	VAL	3.5
1	I	74	GLU	3.5
1	A	59	LYS	3.4
2	N	256	ILE	3.4
2	M	409	ARG	3.4
1	B	9	ILE	3.4
2	L	28	ALA	3.4
2	N	202	SER	3.4
2	F	296	GLU	3.4
2	M	118	PRO	3.4
2	M	383	TYR	3.4
2	M	117	LEU	3.4
2	M	402	ASP	3.4
1	I	44	GLY	3.4
2	D	371	THR	3.4
1	A	161	LYS	3.4
1	I	172	VAL	3.4
1	C	243	LYS	3.4
1	K	194	PRO	3.4
1	I	86	GLY	3.4
2	F	294	ILE	3.4
2	N	119	LEU	3.4
1	A	346	ALA	3.4
1	C	222	GLY	3.4
2	E	365	GLY	3.4
1	B	470	LEU	3.4
2	E	165	ALA	3.4
1	B	12	PRO	3.4
1	I	473	PRO	3.4
2	L	302	GLU	3.4
1	I	518	MET	3.4
1	K	294	MET	3.3
1	C	375	GLU	3.3
1	K	350	TYR	3.3
1	I	166	TYR	3.3
2	E	453	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	76	GLY	3.3
1	C	192	ALA	3.3
1	J	494	PHE	3.3
2	L	278	PRO	3.3
2	M	307	SER	3.3
1	C	405	ALA	3.3
1	B	210	ARG	3.3
2	N	205	ILE	3.3
1	A	1	MET	3.3
2	F	189	VAL	3.3
1	I	233	GLY	3.3
2	F	156	SER	3.3
1	A	19	MET	3.3
1	K	173	VAL	3.3
1	A	47	ALA	3.3
1	B	367	LYS	3.3
2	L	281	ARG	3.3
2	N	419	GLU	3.3
1	B	113	ARG	3.3
2	L	417	ALA	3.3
1	J	206	LEU	3.3
2	F	79	VAL	3.3
2	L	78	ASP	3.3
2	F	350	PRO	3.3
1	K	172	VAL	3.3
1	B	553	TYR	3.3
1	I	40	ILE	3.3
1	I	91	LEU	3.3
1	K	118	ALA	3.3
1	C	85	ASP	3.3
1	I	297	ALA	3.2
2	F	88	MET	3.2
2	N	85	SER	3.2
1	K	203	THR	3.2
4	H	23	ALA	3.2
2	F	421	PHE	3.2
1	C	270	PRO	3.2
1	K	298	ALA	3.2
1	K	289	ALA	3.2
2	N	206	GLN	3.2
2	N	165	ALA	3.2
2	N	112	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	J	266	LEU	3.2
1	K	572	GLY	3.2
1	I	22	ALA	3.2
2	N	430	ARG	3.2
2	F	244	TYR	3.2
2	F	364	ASN	3.2
1	A	376	GLY	3.2
1	C	66	SER	3.2
1	I	474	ASP	3.2
2	M	401	GLU	3.2
1	I	160	VAL	3.2
2	E	193	ALA	3.2
1	C	109	HIS	3.2
1	C	576	ALA	3.2
1	I	345	PRO	3.2
1	A	14	VAL	3.2
1	K	142	GLY	3.2
1	B	494	PHE	3.2
1	I	162	PRO	3.2
2	M	86	LYS	3.2
1	K	242	ALA	3.2
2	M	403	ALA	3.1
1	B	388	GLY	3.1
1	C	196	GLN	3.1
1	K	290	ASN	3.1
1	K	432	THR	3.1
2	F	34	ASP	3.1
1	C	108	VAL	3.1
1	B	58	LEU	3.1
2	F	362	MET	3.1
1	A	168	VAL	3.1
1	I	32	GLU	3.1
2	D	45	GLY	3.1
2	N	349	TYR	3.1
1	K	469	GLN	3.1
2	E	164	ALA	3.1
1	I	75	LEU	3.1
1	C	65	VAL	3.1
1	I	497	GLN	3.1
2	F	242	ALA	3.1
2	F	216	ARG	3.1
2	N	421	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	575	LYS	3.1
2	N	144	LEU	3.1
1	C	184	TYR	3.1
2	E	87	GLU	3.1
2	M	146	ARG	3.1
2	L	346	LYS	3.1
2	L	301	VAL	3.1
1	J	520	LEU	3.1
1	I	365	ALA	3.1
1	I	519	ILE	3.1
2	D	44	GLY	3.1
2	F	402	ASP	3.1
1	I	554	VAL	3.1
1	K	240	SER	3.1
1	K	344	MET	3.1
1	I	315	ASP	3.1
2	D	445	MET	3.0
1	J	128	GLU	3.0
2	F	243	GLU	3.0
1	J	3	GLN	3.0
1	K	43	ASP	3.0
2	D	116	GLY	3.0
2	F	248	GLU	3.0
1	C	201	PRO	3.0
1	I	19	MET	3.0
1	I	219	ALA	3.0
2	D	29	TYR	3.0
1	K	193	ARG	3.0
2	F	12	THR	3.0
2	N	336	GLN	3.0
1	B	77	PRO	3.0
2	D	77	GLU	3.0
2	M	442	LEU	3.0
1	K	314	ARG	3.0
1	K	433	SER	3.0
1	B	59	LYS	3.0
1	I	485	GLU	3.0
2	D	76	VAL	3.0
1	I	344	MET	3.0
2	F	83	GLY	3.0
1	K	530	ILE	3.0
2	D	205	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
2	M	128	GLU	3.0
2	F	63	THR	3.0
4	H	98	ILE	3.0
1	B	108	VAL	3.0
1	B	387	PRO	3.0
2	F	80	ALA	3.0
1	B	517	LYS	3.0
1	C	179	THR	3.0
2	M	171	ALA	3.0
2	N	432	ILE	3.0
1	I	552	ARG	3.0
1	C	72	ALA	3.0
2	F	157	GLY	3.0
1	C	151	PRO	3.0
1	C	288	ILE	3.0
2	F	205	ILE	3.0
1	J	474	ASP	2.9
1	I	161	LYS	2.9
1	A	194	PRO	2.9
1	K	241	LEU	2.9
2	F	278	PRO	2.9
2	L	382	LEU	2.9
4	H	66	ARG	2.9
2	N	9	THR	2.9
1	C	199	LEU	2.9
2	F	10	GLY	2.9
1	K	186	THR	2.9
2	M	81	ARG	2.9
1	A	44	GLY	2.9
2	L	421	PHE	2.9
2	N	65	GLY	2.9
2	F	64	THR	2.9
1	C	274	ASP	2.9
1	B	559	PHE	2.9
1	B	183	MET	2.9
1	C	198	LYS	2.9
4	P	84	HIS	2.9
2	M	365	GLY	2.9
2	N	184	GLU	2.9
2	N	335	GLY	2.9
1	I	170	GLU	2.9
1	B	78	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	I	354	LEU	2.9
2	D	18	LEU	2.9
1	A	210	ARG	2.9
1	A	404	GLY	2.9
1	K	574	PHE	2.9
1	B	214	VAL	2.9
2	E	174	ARG	2.9
2	F	225	ASP	2.9
2	M	131	ILE	2.9
1	C	360	ALA	2.9
2	F	341	ARG	2.9
1	A	108	VAL	2.9
1	K	394	PRO	2.9
2	M	169	ARG	2.8
2	L	96	ILE	2.8
2	M	412	LEU	2.8
2	D	132	GLN	2.8
1	I	478	ASP	2.8
1	B	222	GLY	2.8
1	J	346	ALA	2.8
2	E	378	VAL	2.8
1	C	501	HIS	2.8
1	I	543	PRO	2.8
1	I	355	ALA	2.8
1	B	531	LYS	2.8
1	I	376	GLY	2.8
2	M	311	ILE	2.8
2	N	24	ALA	2.8
2	D	450	GLU	2.8
1	I	312	TYR	2.8
4	H	64	ARG	2.8
1	B	218	VAL	2.8
1	I	31	GLY	2.8
2	E	439	ALA	2.8
2	D	14	ILE	2.8
2	N	255	VAL	2.8
2	N	278	PRO	2.8
1	B	519	ILE	2.8
1	K	44	GLY	2.8
1	I	538	GLU	2.8
2	E	135	ILE	2.8
1	K	470	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
2	N	296	GLU	2.8
1	A	217	PRO	2.8
2	N	167	ILE	2.8
2	M	363	ASN	2.8
1	A	46	THR	2.8
1	A	577	LEU	2.8
2	N	97	GLY	2.8
1	I	475	ALA	2.8
2	F	366	VAL	2.8
1	A	148	LEU	2.7
1	A	192	ALA	2.7
2	N	12	THR	2.7
1	K	293	ASN	2.7
2	M	144	LEU	2.7
1	A	202	ASN	2.7
1	C	277	THR	2.7
1	I	58	LEU	2.7
2	N	279	GLY	2.7
1	I	567	MET	2.7
1	I	175	LEU	2.7
2	D	15	SER	2.7
2	N	366	VAL	2.7
1	K	509	MET	2.7
1	A	224	ALA	2.7
2	N	295	TYR	2.7
1	K	266	LEU	2.7
2	N	239	LEU	2.7
2	D	21	VAL	2.7
2	N	454	ILE	2.7
2	N	309	THR	2.7
2	M	123	ALA	2.7
2	F	117	LEU	2.7
2	L	461	LYS	2.7
2	M	69	ALA	2.7
1	J	560	PRO	2.7
1	A	507	CYS	2.7
1	I	544	VAL	2.7
1	K	191	ARG	2.7
1	I	69	LEU	2.7
1	I	476	LEU	2.7
1	J	562	TYR	2.7
2	D	61	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	J	528	ALA	2.7
1	I	20	LEU	2.7
1	I	120	THR	2.7
1	I	171	PRO	2.7
2	M	235	PRO	2.7
2	E	336	GLN	2.7
2	L	280	ARG	2.7
2	L	260	MET	2.7
1	C	353	TYR	2.7
1	B	11	GLY	2.7
1	I	313	PHE	2.6
2	N	201	LEU	2.6
2	D	130	PHE	2.6
2	N	199	ARG	2.6
1	K	141	PHE	2.6
1	C	378	VAL	2.6
2	E	454	ILE	2.6
1	I	259	GLY	2.6
2	N	170	GLN	2.6
2	L	400	GLY	2.6
1	C	346	ALA	2.6
1	K	52	TYR	2.6
2	D	401	GLU	2.6
2	M	334	GLU	2.6
1	I	110	ALA	2.6
1	I	486	VAL	2.6
2	N	188	ALA	2.6
1	C	87	ILE	2.6
1	C	344	MET	2.6
1	K	192	ALA	2.6
1	J	12	PRO	2.6
1	A	175	LEU	2.6
1	J	58	LEU	2.6
1	K	549	GLY	2.6
2	E	70	THR	2.6
2	N	185	GLU	2.6
2	L	399	ILE	2.6
1	K	174	VAL	2.6
2	F	74	SER	2.6
2	N	411	TYR	2.6
1	I	364	ARG	2.6
2	E	333	THR	2.5

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Mol	Chain	Res	Type	RSRZ
2	M	126	LYS	2.5
1	B	215	LEU	2.5
2	F	35	ILE	2.5
2	L	95	GLY	2.5
1	K	382	GLY	2.5
2	L	81	ARG	2.5
1	A	157	VAL	2.5
1	I	556	GLU	2.5
2	E	376	LYS	2.5
1	A	559	PHE	2.5
2	D	452	LYS	2.5
2	F	363	ASN	2.5
2	F	29	TYR	2.5
2	E	326	PRO	2.5
1	I	548	ILE	2.5
2	L	300	VAL	2.5
2	N	25	LYS	2.5
1	B	10	ALA	2.5
1	I	537	ASP	2.5
1	J	551	ALA	2.5
1	J	267	VAL	2.5
1	J	210	ARG	2.5
2	E	363	ASN	2.5
2	L	224	ALA	2.5
2	N	365	GLY	2.5
2	N	18	LEU	2.5
1	B	16	ALA	2.5
1	I	47	ALA	2.5
2	E	21	VAL	2.5
2	L	298	ALA	2.5
1	A	64	VAL	2.5
1	K	570	ILE	2.5
2	F	342	GLU	2.5
1	K	571	GLN	2.5
1	A	551	ALA	2.5
1	C	200	ASP	2.5
2	N	383	TYR	2.5
1	A	552	ARG	2.5
1	A	375	GLU	2.5
2	D	297	ARG	2.5
2	M	150	LEU	2.5
2	N	108	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
2	L	44	GLY	2.5
1	A	45	ASP	2.5
2	E	364	ASN	2.5
2	N	145	VAL	2.5
2	M	445	MET	2.5
1	K	529	ALA	2.5
2	L	229	ILE	2.5
1	K	88	GLN	2.4
2	M	120	ASN	2.4
1	I	45	ASP	2.4
2	D	288	TYR	2.4
2	N	423	ILE	2.4
1	A	560	PRO	2.4
2	M	426	GLY	2.4
1	I	401	ARG	2.4
1	I	484	ILE	2.4
1	I	83	ILE	2.4
1	K	158	LYS	2.4
2	N	35	ILE	2.4
1	A	60	VAL	2.4
1	A	344	MET	2.4
2	D	439	ALA	2.4
2	L	55	ALA	2.4
1	A	113	ARG	2.4
1	K	381	VAL	2.4
1	K	140	GLU	2.4
2	E	452	LYS	2.4
1	C	111	LEU	2.4
2	D	59	VAL	2.4
2	E	329	THR	2.4
1	B	242	ALA	2.4
1	C	224	ALA	2.4
2	D	298	ALA	2.4
1	C	268	GLU	2.4
2	D	446	LEU	2.4
1	A	435	LEU	2.4
1	K	66	SER	2.4
1	A	259	GLY	2.4
2	E	81	ARG	2.4
1	I	256	GLY	2.4
2	E	334	GLU	2.4
1	C	193	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
2	N	96	ILE	2.4
1	J	558	GLU	2.4
2	N	382	LEU	2.4
3	G	54	ASP	2.4
4	H	65	GLY	2.4
2	E	69	ALA	2.4
1	I	565	GLU	2.4
2	E	304	LYS	2.4
1	C	76	GLY	2.4
3	O	27	LEU	2.3
2	F	419	GLU	2.3
4	H	63	MET	2.3
2	N	424	ASN	2.3
4	H	25	SER	2.3
2	M	254	LEU	2.3
1	I	70	PRO	2.3
4	P	89	TYR	2.3
2	E	194	MET	2.3
2	F	429	ASN	2.3
1	K	53	GLU	2.3
1	A	79	MET	2.3
1	J	495	LEU	2.3
1	A	63	PRO	2.3
1	J	218	VAL	2.3
2	M	83	GLY	2.3
1	I	535	SER	2.3
2	L	215	SER	2.3
1	A	5	VAL	2.3
1	B	558	GLU	2.3
2	F	221	LEU	2.3
1	I	555	SER	2.3
1	J	493	ASP	2.3
1	I	425	ASN	2.3
2	E	449	GLY	2.3
2	F	120	ASN	2.3
2	N	200	GLU	2.3
2	E	461	LYS	2.3
1	C	5	VAL	2.3
1	I	400	LEU	2.3
1	K	246	ASN	2.3
1	J	57	GLY	2.3
2	L	296	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
2	E	84	VAL	2.3
2	N	308	VAL	2.3
1	B	464	LEU	2.3
1	C	394	PRO	2.3
2	N	381	GLN	2.3
4	H	30	GLN	2.3
1	B	13	ALA	2.3
2	L	297	ARG	2.3
1	J	129	VAL	2.3
1	C	10	ALA	2.2
1	C	88	GLN	2.2
2	M	411	TYR	2.2
1	K	109	HIS	2.2
2	D	62	GLU	2.2
1	K	352	PRO	2.2
2	L	416	ASP	2.2
1	C	359	ALA	2.2
1	I	299	ARG	2.2
2	L	225	ASP	2.2
1	J	349	GLY	2.2
1	A	42	LEU	2.2
1	K	219	ALA	2.2
1	I	129	VAL	2.2
1	I	121	PRO	2.2
2	E	332	ILE	2.2
1	C	175	LEU	2.2
1	K	367	LYS	2.2
1	K	416	ARG	2.2
1	K	243	LYS	2.2
1	A	228	GLY	2.2
1	I	547	ARG	2.2
2	E	382	LEU	2.2
2	L	40	GLY	2.2
2	N	420	ARG	2.2
1	J	478	ASP	2.2
1	K	116	LYS	2.2
2	M	439	ALA	2.2
2	M	130	PHE	2.2
2	F	31	ALA	2.2
1	I	55	THR	2.2
2	N	143	THR	2.2
1	A	225	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	16	GLY	2.2
1	I	481	ARG	2.2
1	J	183	MET	2.2
4	P	74	ILE	2.2
1	I	495	LEU	2.2
2	E	73	VAL	2.2
1	C	273	THR	2.2
1	J	194	PRO	2.2
4	P	98	ILE	2.2
2	D	436	LEU	2.2
1	I	149	VAL	2.2
1	K	386	PRO	2.2
1	K	162	PRO	2.2
1	J	529	ALA	2.2
2	F	188	ALA	2.2
2	D	310	GLN	2.2
2	N	426	GLY	2.2
1	B	554	VAL	2.1
1	J	512	ALA	2.1
2	D	447	PRO	2.1
2	L	33	VAL	2.1
1	I	539	ILE	2.1
2	D	63	THR	2.1
2	L	371	THR	2.1
4	P	1	MET	2.1
1	I	48	PHE	2.1
2	L	25	LYS	2.1
2	N	240	THR	2.1
1	I	184	TYR	2.1
1	I	368	VAL	2.1
2	F	241	VAL	2.1
2	F	24	ALA	2.1
1	A	7	GLN	2.1
1	I	167	THR	2.1
1	I	123	VAL	2.1
1	K	245	SER	2.1
2	L	186	PRO	2.1
2	D	443	LEU	2.1
2	N	455	SER	2.1
1	J	77	PRO	2.1
2	E	29	TYR	2.1
2	F	273	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
2	F	71	THR	2.1
1	K	547	ARG	2.1
2	M	174	ARG	2.1
1	J	366	GLY	2.1
1	K	239	GLN	2.1
1	A	229	PRO	2.1
1	I	295	PRO	2.1
1	I	423	ASN	2.1
1	J	553	TYR	2.1
1	I	85	ASP	2.1
2	E	151	PRO	2.1
1	A	50	GLN	2.1
2	E	72	SER	2.1
2	L	420	ARG	2.1
1	B	204	PRO	2.1
1	I	90	PRO	2.1
2	F	60	PHE	2.1
2	F	70	THR	2.1
2	F	158	LEU	2.1
2	F	201	LEU	2.1
1	K	271	GLU	2.1
2	E	307	SER	2.1
2	N	237	MET	2.1
2	N	370	LYS	2.1
1	I	405	ALA	2.1
1	K	388	GLY	2.1
2	M	67	ASP	2.1
2	L	221	LEU	2.1
2	D	222	ASN	2.1
1	I	351	PRO	2.1
2	N	203	TYR	2.1
1	A	65	VAL	2.1
1	B	211	ILE	2.1
1	B	532	ARG	2.1
1	K	445	GLU	2.1
3	G	136	ALA	2.1
2	N	116	GLY	2.1
1	C	289	ALA	2.1
2	M	88	MET	2.1
2	L	226	ASP	2.1
2	E	55	ALA	2.1
2	F	348	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	574	PHE	2.1
1	B	248	ASP	2.1
1	K	349	GLY	2.1
2	F	324	PRO	2.1
1	C	219	ALA	2.1
1	I	201	PRO	2.1
1	B	217	PRO	2.0
1	K	537	ASP	2.0
2	D	34	ASP	2.0
2	N	34	ASP	2.0
1	A	88	GLN	2.0
1	B	219	ALA	2.0
2	D	193	ALA	2.0
2	E	28	ALA	2.0
1	C	349	GLY	2.0
1	C	181	LEU	2.0
1	K	237	THR	2.0
1	I	549	GLY	2.0
2	M	147	GLY	2.0
2	N	88	MET	2.0
1	I	399	THR	2.0
2	N	29	TYR	2.0
2	N	171	ALA	2.0
2	L	115	THR	2.0
1	J	531	LYS	2.0
2	F	422	PHE	2.0
1	C	190	ARG	2.0
2	D	60	PHE	2.0
1	I	436	ASP	2.0
1	A	366	GLY	2.0
2	F	420	ARG	2.0
1	B	221	GLY	2.0
1	J	552	ARG	2.0
2	D	451	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.