



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2024 – 12:58 AM EST

PDB ID : 3SYV
Title : Crystal structure of mPACSIN 3 F-BAR domain mutant
Authors : Bai, X.
Deposited on : 2011-07-18
Resolution : 3.10 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

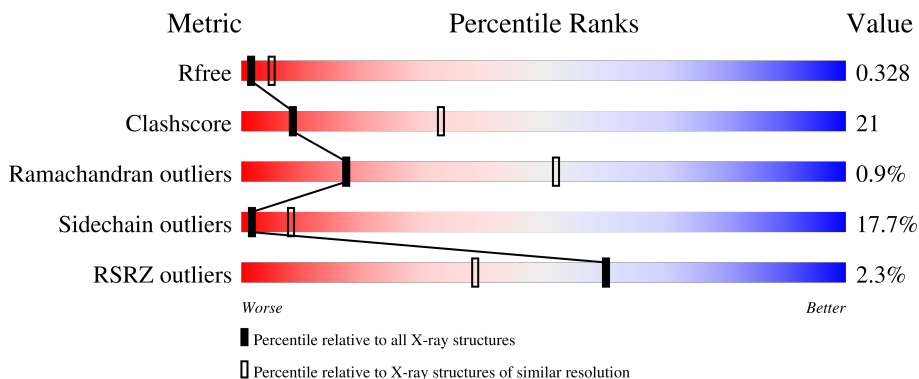
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

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



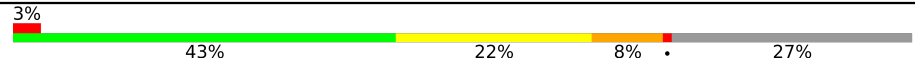
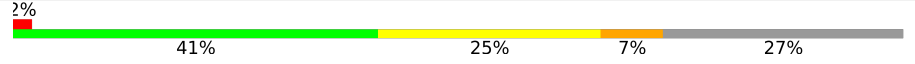
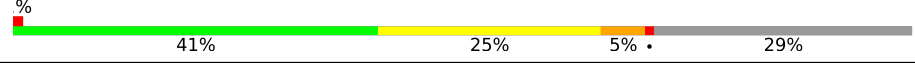
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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

Mol	Chain	Length	Quality of chain
1	A	347	
1	B	347	
1	C	347	
1	D	347	
1	E	347	

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Mol	Chain	Length	Quality of chain
1	F	347	 <p>3% 43% 22% 8% 27%</p>
1	G	347	 <p>2% 41% 25% 7% 27%</p>
1	H	347	 <p>% 41% 25% 5% 29%</p>

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 16470 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Protein kinase C and casein kinase II substrate protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	250	Total 2047	C 1284	N 384	O 372	S 7	0	0	0
1	B	257	Total 2115	C 1317	N 403	O 387	S 8	0	0	0
1	C	257	Total 2061	C 1284	N 390	O 379	S 8	0	0	0
1	D	255	Total 2085	C 1304	N 396	O 378	S 7	0	0	0
1	E	255	Total 2044	C 1278	N 387	O 374	S 5	0	0	1
1	F	255	Total 2050	C 1283	N 392	O 369	S 6	0	0	0
1	G	254	Total 1978	C 1231	N 374	O 368	S 5	0	0	0
1	H	247	Total 1981	C 1236	N 378	O 364	S 3	0	0	0

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	expression tag	UNP Q99JB8
A	-4	HIS	-	expression tag	UNP Q99JB8
A	-3	HIS	-	expression tag	UNP Q99JB8
A	-2	HIS	-	expression tag	UNP Q99JB8
A	-1	HIS	-	expression tag	UNP Q99JB8
A	0	HIS	-	expression tag	UNP Q99JB8
A	121	GLN	PRO	engineered mutation	UNP Q99JB8
B	-5	HIS	-	expression tag	UNP Q99JB8
B	-4	HIS	-	expression tag	UNP Q99JB8
B	-3	HIS	-	expression tag	UNP Q99JB8
B	-2	HIS	-	expression tag	UNP Q99JB8
B	-1	HIS	-	expression tag	UNP Q99JB8
B	0	HIS	-	expression tag	UNP Q99JB8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	121	GLN	PRO	engineered mutation	UNP Q99JB8
C	-5	HIS	-	expression tag	UNP Q99JB8
C	-4	HIS	-	expression tag	UNP Q99JB8
C	-3	HIS	-	expression tag	UNP Q99JB8
C	-2	HIS	-	expression tag	UNP Q99JB8
C	-1	HIS	-	expression tag	UNP Q99JB8
C	0	HIS	-	expression tag	UNP Q99JB8
C	121	GLN	PRO	engineered mutation	UNP Q99JB8
D	-5	HIS	-	expression tag	UNP Q99JB8
D	-4	HIS	-	expression tag	UNP Q99JB8
D	-3	HIS	-	expression tag	UNP Q99JB8
D	-2	HIS	-	expression tag	UNP Q99JB8
D	-1	HIS	-	expression tag	UNP Q99JB8
D	0	HIS	-	expression tag	UNP Q99JB8
D	121	GLN	PRO	engineered mutation	UNP Q99JB8
E	-5	HIS	-	expression tag	UNP Q99JB8
E	-4	HIS	-	expression tag	UNP Q99JB8
E	-3	HIS	-	expression tag	UNP Q99JB8
E	-2	HIS	-	expression tag	UNP Q99JB8
E	-1	HIS	-	expression tag	UNP Q99JB8
E	0	HIS	-	expression tag	UNP Q99JB8
E	121	GLN	PRO	engineered mutation	UNP Q99JB8
F	-5	HIS	-	expression tag	UNP Q99JB8
F	-4	HIS	-	expression tag	UNP Q99JB8
F	-3	HIS	-	expression tag	UNP Q99JB8
F	-2	HIS	-	expression tag	UNP Q99JB8
F	-1	HIS	-	expression tag	UNP Q99JB8
F	0	HIS	-	expression tag	UNP Q99JB8
F	121	GLN	PRO	engineered mutation	UNP Q99JB8
G	-5	HIS	-	expression tag	UNP Q99JB8
G	-4	HIS	-	expression tag	UNP Q99JB8
G	-3	HIS	-	expression tag	UNP Q99JB8
G	-2	HIS	-	expression tag	UNP Q99JB8
G	-1	HIS	-	expression tag	UNP Q99JB8
G	0	HIS	-	expression tag	UNP Q99JB8
G	121	GLN	PRO	engineered mutation	UNP Q99JB8
H	-5	HIS	-	expression tag	UNP Q99JB8
H	-4	HIS	-	expression tag	UNP Q99JB8
H	-3	HIS	-	expression tag	UNP Q99JB8
H	-2	HIS	-	expression tag	UNP Q99JB8
H	-1	HIS	-	expression tag	UNP Q99JB8
H	0	HIS	-	expression tag	UNP Q99JB8

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Chain	Residue	Modelled	Actual	Comment	Reference
H	121	GLN	PRO	engineered mutation	UNP Q99JB8

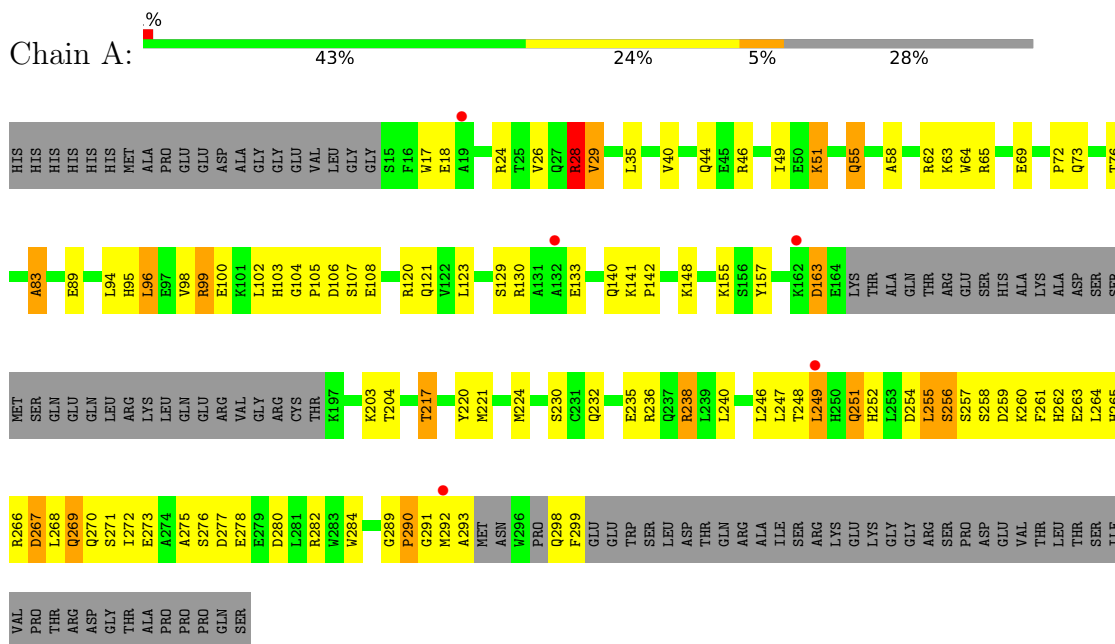
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	14	Total O 14 14	0	0
2	B	13	Total O 13 13	0	0
2	C	19	Total O 19 19	0	0
2	D	12	Total O 12 12	0	0
2	E	12	Total O 12 12	0	0
2	F	16	Total O 16 16	0	0
2	G	10	Total O 10 10	0	0
2	H	13	Total O 13 13	0	0

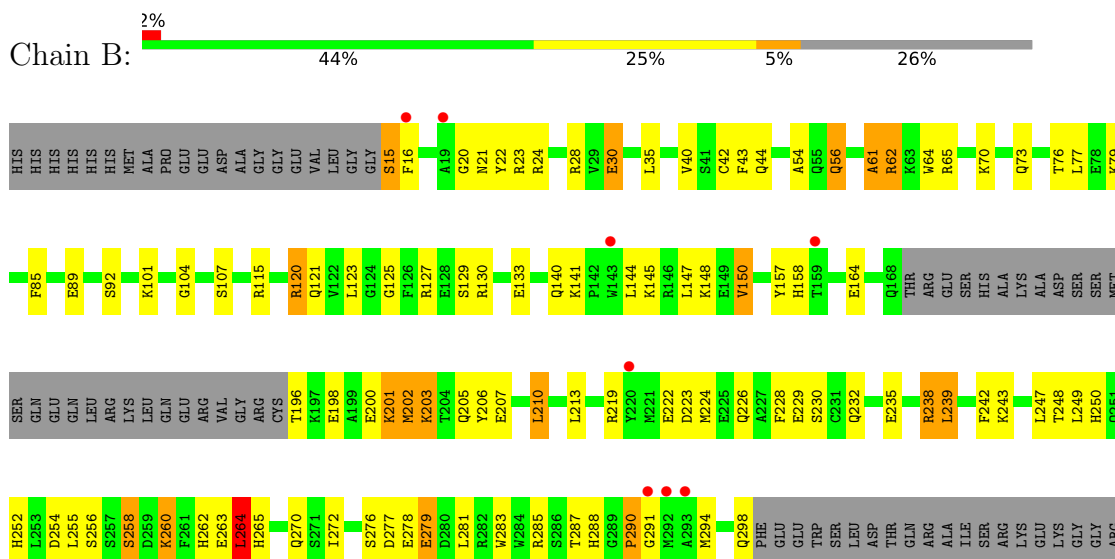
3 Residue-property plots

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

- Molecule 1: Protein kinase C and casein kinase II substrate protein 3



- Molecule 1: Protein kinase C and casein kinase II substrate protein 3



SER
PRO
ASP
GLU
VAL
THR
LEU
THR
SER
SER
VAL
ILE
VAL
PRO
THR
ARG
ASP
GLY
THR
ALA
PRO
PRO
PRO
GLN
GLN
SER

● Molecule 1: Protein kinase C and casein kinase II substrate protein 3



HIS
HIS
HIS
HIS
HIS
HIS
HIS
MET
ALA
PRO
GLU
LEU
ASP
ALA
G8
G14
S15
F16
W17
E18
A19
G20
N21
Y22
R23
R24
T25
V26
R28
V29
E30
D31
R34
L35
C36
V40
Q44
E45
Q56
L57
A58
G71
P72
Q73
T76
K79

A80
W81
A83
F84
F85
T86
E89
R90
E93
R99
E100
K101
E108
Q114
R130
R137
Q140
K141
P142
W143
L144
K145
R146
L147
R34
E149
L35
C36
V40
S153
K154
Q156
S156
Y157
H158
T159
D163
GLU
LYS
THR
ALA
GLN
THR
ARG
GLU
HIS
ALA
LYS
ALA
ASP

SER
SER
MET
SER
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LEU
ARG
VAL
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GLU
GLN
ARG
VAL
GLY
CYS
THR
LYS
E198
A199
E200
N201
M202
K203
T204
Q205
P142
W143
E206
Y207
E207
Q208
T209
L210
A211
E212
L213
N214
R215
Y216
T217
P218
R219
Y220
M221
M224
A227
F228
Q232
E235
R238
D244
V245
L246
L247

Q251
R252
L253
D254
L255
S256
S257
D259
K260
F261
H262
E263
H264
H265
R266
D267
L268
Q269
Q270
S271
L272
L273
E274
A275
S276
D277
E278
E279
D280
L281
W284
R285
G289
F289
G291
M292
A293
M294
N295
Y296
PRO
Q299
F299
GLU
GLY
TRP
SER
LEU
THR
ASP
GLN
ARG
ALA
ILE
SER
ARG

LYS
GLU
LYS
GLY
GLY
ARG
SER
PRO
ASP
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SER
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VAL
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ASP
GLY
ALA
PRO
PRO
GLN
SER

● Molecule 1: Protein kinase C and casein kinase II substrate protein 3



HIS
HIS
HIS
HIS
HIS
HIS
MET
ALA
PRO
GLU
GLU
ASP
ALA
GLY
S15
F16
W17
E18
G20
N21
Y22
R23
R24
R28
R34
L35
D38
L39
V40
F43
Q44
A47
R48
L49
E50
K51
Q56
R62
R63
W64
R65
G66
A67
V68
E69
K70

G71
P72
T76
L77
W81
F84
E89
R90
E93
L94
H95
V98
R99
E100
K101
L102
D106
S107
E108
R109
V110
H119
R120
Q121
G124
G125
F126
R127
R130
E133
Q44
Q140
W143
L147
K148
E151
H158
T159
A160
R161
E164
K165
THR
ALA

GLN
THR
ARG
GLU
SER
HIS
ALA
LYS
ALA
ASP
GLU
SER
MET
SER
SER
GLN
GLU
GLN
LEU
ARG
LYS
LEU
GLY
L102
D106
S107
E108
R109
V110
H119
R120
Q121
G124
G125
F126
R127
R130
E133
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K148
E151
H158
T159
A160
R161
E164
K165
THR
ALA

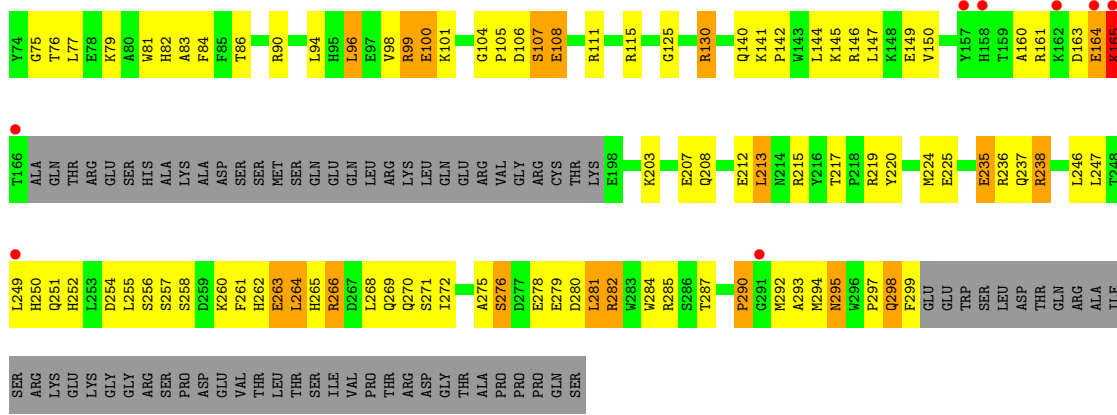
R236
Q237
L239
K243
D244
V245
L247
L248
L249
H250
L255
S256
S257
S258
D259
K260
F261
R266
Q269
A275
S276
D277
E278
E279
D280
L281
R282
S285
T287
H288
G289
P290
C291
M292
ALA
M294
Q298
F299
GLU
TRP
M224
E225
Q226
A227
F228
C231
Q232
E235

ARG
LYS
GLU
LYS
GLY
ARG
SER
PRO
ASP
GLU
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THR
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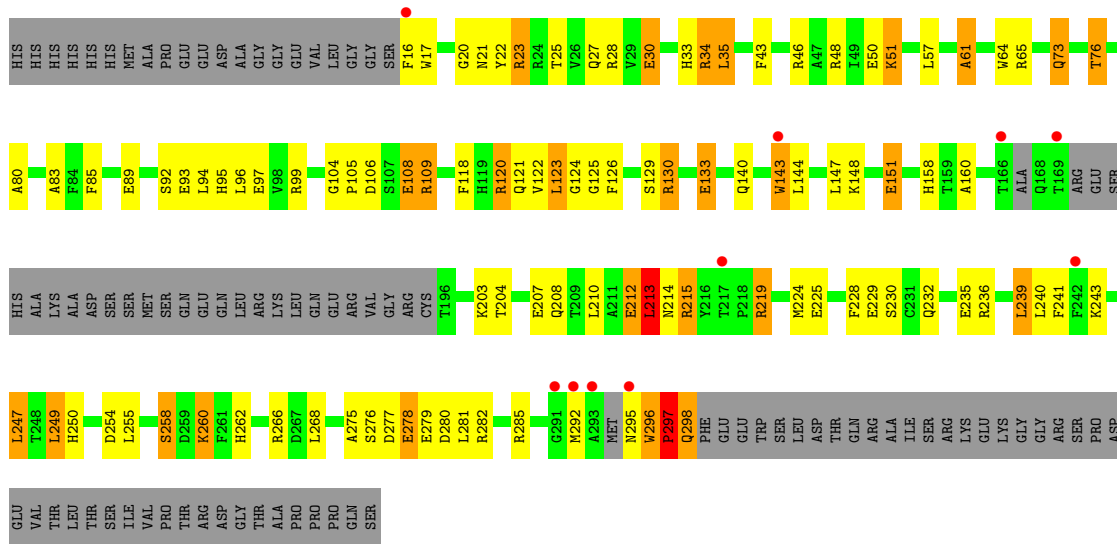
● Molecule 1: Protein kinase C and casein kinase II substrate protein 3



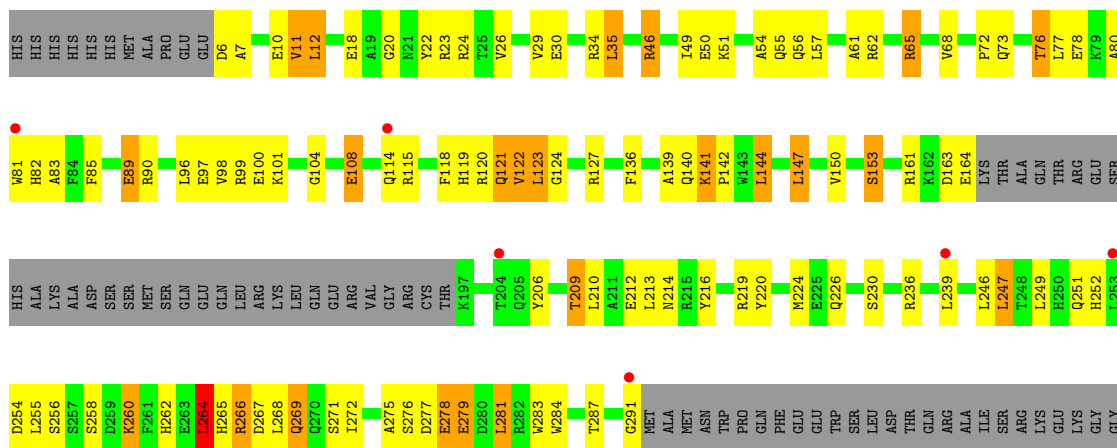
HIS
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G14
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F16
W17
E18
A19
G20
N21
Y22
R23
R24
R28
V29
E30
R34
L35
V40
S41
C42
F43
Q44
A47
E50
Q55
R62
K63
W64
R65
E69
K70
P72
G71
Q73



• Molecule 1: Protein kinase C and casein kinase II substrate protein 3



• Molecule 1: Protein kinase C and casein kinase II substrate protein 3



ARG
SER
PRO
ASP
GLU
VAL
THR
LEU
THR
SER
ILE
VAL
PRO
THR
ARG
ASP
GLY
THR
ALA
PRO
PRO
PRO
GLN
GLN
SER

• Molecule 1: Protein kinase C and casein kinase II substrate protein 3

Chain H: 41% 25% 5% 29%

HIS
HIS
HIS
HIS
HIS
HIS
MET
ALA
PRO
GLU
GLU
ILE
ASP
ALA
GLY
GLY
VAL
LEU
GLY
G14
S15
F16
W17
W17
E18
A19
G20
R23
R24
R28
Y28
E30
D31
L35
C36
L38
V40
S41
A47
R48
I49
E50
K51
A54
Q55
Q56
L57
R62
K63
W64
A67
V68
E69

K70
G71
Q73
T76
L77
W81
H82
F85
A88
E89
R90
L91
S92
E93
L94
H95
L96
E97
V98
R99
E100
G104
P105
D106
S107
E108
R109
V110
R115
R120
Q121
R127
R130
K141
P142
W143
L144
L147
A160
E164
LYS
THR
ALA
GLN
THR
ARG

GLU
SER
HIS
ALA
LYS
ALA
ASP
SER
SER
MET
SER
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GLN
LEU
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LYS
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GLN
GLU
ARG
VAL
GLY
ARG
G195
K203
T204
Q205
Y206
E207
Q208
T209
L210
Y216
THR
P218
R219
E225
F228
E229
S230
C231
Q232
E235
R236
Q237
R238
L239
F242
K243
L247
T248
L249

H250
Q251
H252
L253
D254
S258
D259
K260
F261
L264
H265
R266
Q269
A275
S276
D277
E278
E279
D280
L281
S286
T287
H288
G289
P290
G291
MET
ALA
MET
ASN
TRP
PRO
GLN
PHE
GLU
GLU
TRP
SER
LEU
ASP
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ALA
ILE
SER
ARG
LYS
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GLY
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ASP
GLU
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LEU
THR
SER
ILE
VAL
PRO
THR
THR
ARG
ASP
GLY
THR
ALA
PRO
PRO
GLN
GLN
SER

4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	120.57Å 108.90Å 222.32Å 90.00° 90.05° 90.00°	Depositor
Resolution (Å)	48.90 – 3.10 48.90 – 3.10	Depositor EDS
% Data completeness (in resolution range)	98.7 (48.90-3.10) 98.5 (48.90-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.60 (at 3.12Å)	Xtrriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.281 , 0.337 0.274 , 0.328	Depositor DCC
R_{free} test set	5196 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	64.1	Xtrriage
Anisotropy	0.371	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 31.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.55$, $\langle L^2 \rangle = 0.40$	Xtrriage
Estimated twinning fraction	0.458 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	16470	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 50.83 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.1201e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.12	6/2094 (0.3%)	1.01	5/2811 (0.2%)
1	B	1.14	7/2160 (0.3%)	1.00	2/2895 (0.1%)
1	C	1.12	8/2104 (0.4%)	1.00	4/2821 (0.1%)
1	D	1.26	11/2133 (0.5%)	1.06	4/2862 (0.1%)
1	E	1.17	6/2092 (0.3%)	1.02	6/2813 (0.2%)
1	F	1.22	12/2097 (0.6%)	1.05	2/2821 (0.1%)
1	G	1.14	3/2021 (0.1%)	1.03	5/2724 (0.2%)
1	H	1.28	12/2025 (0.6%)	1.08	9/2725 (0.3%)
All	All	1.18	65/16726 (0.4%)	1.03	37/22472 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	108	GLU	CG-CD	10.46	1.67	1.51
1	H	108	GLU	CG-CD	10.14	1.67	1.51
1	D	160	ALA	C-O	9.96	1.42	1.23
1	H	97	GLU	CG-CD	9.93	1.66	1.51
1	A	108	GLU	CG-CD	8.23	1.64	1.51
1	A	100	GLU	CG-CD	7.84	1.63	1.51
1	D	161	ARG	CZ-NH1	7.74	1.43	1.33
1	F	30	GLU	CG-CD	7.66	1.63	1.51
1	E	108	GLU	CG-CD	7.66	1.63	1.51
1	H	160	ALA	C-O	7.38	1.37	1.23
1	D	196	THR	CB-CG2	7.29	1.76	1.52
1	H	290	PRO	N-CA	6.72	1.58	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	160	ALA	C-O	6.69	1.36	1.23
1	F	97	GLU	CD-OE1	6.67	1.32	1.25
1	F	120	ARG	CG-CD	6.59	1.68	1.51
1	D	285	ARG	CG-CD	6.52	1.68	1.51
1	E	100	GLU	CG-CD	6.43	1.61	1.51
1	C	156	SER	C-O	6.39	1.35	1.23
1	F	97	GLU	CD-OE2	6.35	1.32	1.25
1	C	24	ARG	CG-CD	6.34	1.67	1.51
1	H	18	GLU	CG-CD	6.34	1.61	1.51
1	D	148	LYS	CE-NZ	6.30	1.64	1.49
1	B	290	PRO	N-CA	6.30	1.57	1.47
1	D	69	GLU	CG-CD	6.26	1.61	1.51
1	G	124	GLY	N-CA	6.20	1.55	1.46
1	A	100	GLU	CD-OE2	6.16	1.32	1.25
1	F	279	GLU	CG-CD	6.15	1.61	1.51
1	G	108	GLU	CG-CD	6.06	1.61	1.51
1	H	225	GLU	CD-OE2	6.06	1.32	1.25
1	F	61	ALA	CA-CB	-6.06	1.39	1.52
1	D	165	LYS	CE-NZ	6.00	1.64	1.49
1	H	164	GLU	C-O	5.97	1.34	1.23
1	A	89	GLU	CG-CD	5.92	1.60	1.51
1	D	285	ARG	CD-NE	5.92	1.56	1.46
1	F	215	ARG	CZ-NH2	5.86	1.40	1.33
1	D	70	LYS	CD-CE	5.85	1.65	1.51
1	B	30	GLU	CB-CG	5.84	1.63	1.52
1	H	120	ARG	CG-CD	5.78	1.66	1.51
1	B	145	LYS	CD-CE	5.77	1.65	1.51
1	B	61	ALA	CA-CB	-5.71	1.40	1.52
1	B	263	GLU	CG-CD	5.67	1.60	1.51
1	C	235	GLU	CG-CD	5.60	1.60	1.51
1	E	165	LYS	CE-NZ	5.53	1.62	1.49
1	E	108	GLU	CD-OE1	5.53	1.31	1.25
1	D	17	TRP	CD1-NE1	5.51	1.47	1.38
1	H	100	GLU	CG-CD	5.47	1.60	1.51
1	C	299	PHE	N-CA	5.46	1.57	1.46
1	G	278	GLU	CG-CD	5.45	1.60	1.51
1	F	30	GLU	CB-CG	5.42	1.62	1.52
1	E	108	GLU	CD-OE2	5.37	1.31	1.25
1	H	54	ALA	CA-CB	-5.30	1.41	1.52
1	C	235	GLU	CB-CG	5.23	1.62	1.52
1	B	279	GLU	CG-CD	5.22	1.59	1.51
1	C	141	LYS	CD-CE	5.21	1.64	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	291	GLY	N-CA	5.21	1.53	1.46
1	C	108	GLU	CG-CD	5.19	1.59	1.51
1	C	278	GLU	CG-CD	5.17	1.59	1.51
1	F	266	ARG	CG-CD	5.14	1.64	1.51
1	F	97	GLU	CG-CD	5.14	1.59	1.51
1	D	231	CYS	CB-SG	-5.13	1.73	1.81
1	A	121	GLN	CG-CD	5.11	1.62	1.51
1	B	263	GLU	CB-CG	5.09	1.61	1.52
1	A	121	GLN	CB-CG	5.05	1.66	1.52
1	H	69	GLU	CG-CD	5.02	1.59	1.51
1	E	299	PHE	CA-CB	-5.01	1.43	1.53

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	238	ARG	NE-CZ-NH2	-9.19	115.71	120.30
1	D	161	ARG	NE-CZ-NH2	-7.60	116.50	120.30
1	A	28	ARG	NE-CZ-NH1	6.89	123.75	120.30
1	F	219	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	E	238	ARG	NE-CZ-NH2	-6.84	116.88	120.30
1	E	238	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	G	122	VAL	N-CA-C	-6.39	93.74	111.00
1	C	46	ARG	NE-CZ-NH2	-6.39	117.11	120.30
1	H	127	ARG	NE-CZ-NH2	-6.21	117.19	120.30
1	B	264	LEU	CA-CB-CG	6.20	129.57	115.30
1	A	282	ARG	NE-CZ-NH1	6.17	123.39	120.30
1	H	127	ARG	NE-CZ-NH1	6.13	123.36	120.30
1	H	35	LEU	CB-CG-CD1	6.04	121.26	111.00
1	E	165	LYS	O-C-N	5.96	132.24	122.70
1	C	238	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	C	238	ARG	NE-CZ-NH2	-5.91	117.34	120.30
1	H	99	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	H	115	ARG	NE-CZ-NH1	-5.68	117.46	120.30
1	D	285	ARG	NE-CZ-NH2	5.63	123.11	120.30
1	H	249	LEU	CA-CB-CG	5.61	128.20	115.30
1	A	28	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	D	48	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	G	264	LEU	CA-CB-CG	5.40	127.72	115.30
1	G	123	LEU	CB-CG-CD2	5.37	120.13	111.00
1	G	46	ARG	NE-CZ-NH1	5.35	122.98	120.30
1	E	255	LEU	CA-CB-CG	5.34	127.58	115.30
1	E	213	LEU	CA-CB-CG	5.32	127.54	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	35	LEU	CB-CG-CD2	5.28	119.97	111.00
1	C	224	MET	CG-SD-CE	-5.24	91.82	100.20
1	G	118	PHE	N-CA-C	-5.21	96.94	111.00
1	D	291	GLY	N-CA-C	5.20	126.10	113.10
1	E	282	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	A	249	LEU	CA-CB-CG	-5.12	103.53	115.30
1	B	62	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	F	297	PRO	N-CA-C	-5.10	98.84	112.10
1	H	90	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	H	247	LEU	CA-CB-CG	5.07	126.96	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	160	ALA	Mainchain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2047	0	1943	82	0
1	B	2115	0	2020	76	0
1	C	2061	0	1930	97	0
1	D	2085	0	1982	110	0
1	E	2044	0	1900	111	0
1	F	2050	0	1898	93	0
1	G	1978	0	1807	89	0
1	H	1981	0	1827	84	0
2	A	14	0	0	1	0
2	B	13	0	0	2	0
2	C	19	0	0	0	0
2	D	12	0	0	3	0
2	E	12	0	0	0	0
2	F	16	0	0	2	0
2	G	10	0	0	0	0
2	H	13	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	16470	0	15307	658	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 21.

All (658) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:196:THR:CB	1:D:196:THR:CG2	1.76	1.59
1:D:121:GLN:HE22	1:D:130:ARG:CD	1.42	1.33
1:D:121:GLN:NE2	1:D:130:ARG:HD3	1.46	1.30
1:E:76:THR:CG2	1:E:275:ALA:HA	1.69	1.23
1:A:76:THR:CG2	1:A:275:ALA:HA	1.74	1.18
1:G:276:SER:HB3	1:G:279:GLU:HB2	1.21	1.14
1:B:229:GLU:OE1	1:B:229:GLU:OE2	1.69	1.10
1:D:120:ARG:H	1:D:120:ARG:HD3	1.08	1.09
1:E:76:THR:HG21	1:E:275:ALA:HA	1.28	1.08
1:H:76:THR:CG2	1:H:275:ALA:HA	1.86	1.05
1:H:121:GLN:HE22	1:H:130:ARG:HD2	1.21	1.04
1:H:76:THR:HG21	1:H:275:ALA:HA	1.36	1.02
1:H:216:TYR:C	1:H:218:PRO:HD2	1.78	1.02
1:A:76:THR:HG22	1:A:275:ALA:HA	1.41	1.01
1:A:247:LEU:O	1:A:251:GLN:HG2	1.60	1.00
1:F:260:LYS:HB2	1:F:260:LYS:NZ	1.78	0.99
1:A:76:THR:HG21	1:A:275:ALA:HA	1.45	0.98
1:G:272:ILE:HG21	1:H:247:LEU:HD13	1.44	0.97
1:D:120:ARG:HA	1:D:125:GLY:O	1.64	0.97
1:H:121:GLN:HE22	1:H:130:ARG:CD	1.78	0.97
1:A:235:GLU:CG	1:A:238:ARG:HH21	1.77	0.96
1:C:35:LEU:HD11	1:D:72:PRO:HD2	1.42	0.96
1:D:121:GLN:HE22	1:D:130:ARG:HD3	0.79	0.95
1:D:120:ARG:H	1:D:120:ARG:CD	1.79	0.93
1:E:76:THR:HG22	1:E:275:ALA:HA	1.47	0.92
1:G:276:SER:CB	1:G:279:GLU:HB2	2.00	0.91
1:F:296:TRP:HE3	1:F:296:TRP:N	1.70	0.90
1:H:121:GLN:NE2	1:H:130:ARG:HD2	1.87	0.90
1:C:268:LEU:HD23	1:D:250:HIS:CD2	2.06	0.90
1:F:260:LYS:HB2	1:F:260:LYS:HZ3	1.34	0.90
1:G:65:ARG:NH2	1:G:82:HIS:HB3	1.87	0.90
1:F:151:GLU:OE2	1:F:151:GLU:HA	1.73	0.88
1:C:266:ARG:HH11	1:C:269:GLN:NE2	1.71	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:296:TRP:HE3	1:F:296:TRP:H	0.92	0.88
1:G:20:GLY:HA2	1:G:22:TYR:CE1	2.10	0.87
1:H:31:ASP:O	1:H:35:LEU:HD23	1.76	0.85
1:C:101:LYS:HD2	1:C:252:HIS:CD2	2.12	0.85
1:H:261:PHE:O	1:H:264:LEU:CD2	2.25	0.84
1:C:76:THR:HB	1:C:275:ALA:HA	1.56	0.84
1:F:76:THR:HG23	1:F:275:ALA:HA	1.58	0.84
1:H:264:LEU:HD23	1:H:265:HIS:H	1.43	0.84
1:E:76:THR:HG21	1:E:275:ALA:CA	2.06	0.83
1:C:295:ASN:O	1:C:298:GLN:N	2.11	0.83
1:G:276:SER:HB3	1:G:279:GLU:CB	2.08	0.83
1:E:73:GLN:HE21	1:E:81:TRP:HE3	1.27	0.82
1:C:276:SER:HB3	1:C:279:GLU:HB2	1.61	0.82
1:E:235:GLU:HA	1:E:235:GLU:OE1	1.78	0.82
1:G:163:ASP:CB	1:G:164:GLU:CB	2.59	0.81
1:D:24:ARG:CG	1:D:24:ARG:HH11	1.92	0.81
1:C:228:PHE:HE2	1:C:232:GLN:HE21	1.26	0.81
1:D:282:ARG:HG2	1:D:282:ARG:HH11	1.45	0.80
1:F:123:LEU:H	1:F:123:LEU:HD23	1.46	0.80
1:D:120:ARG:HD3	1:D:120:ARG:N	1.94	0.79
1:A:290:PRO:C	1:A:292:MET:H	1.85	0.79
1:E:268:LEU:HD23	1:F:250:HIS:CD2	2.17	0.79
1:F:76:THR:HB	1:F:280:ASP:OD1	1.83	0.79
1:B:254:ASP:OD1	1:B:256:SER:HB3	1.82	0.78
1:G:163:ASP:CA	1:G:164:GLU:CB	2.61	0.78
1:G:101:LYS:HD2	1:G:252:HIS:CD2	2.18	0.78
1:D:94:LEU:O	1:D:98:VAL:HG23	1.83	0.78
1:D:277:ASP:OD2	1:D:278:GLU:N	2.17	0.78
1:E:71:GLY:HA2	2:F:345:HOH:O	1.82	0.78
1:C:24:ARG:HD3	1:D:288:HIS:ND1	1.99	0.78
1:E:65:ARG:CZ	1:E:82:HIS:HB3	2.14	0.77
1:B:40:VAL:O	1:B:44:GLN:HG3	1.83	0.77
1:G:76:THR:HB	1:G:275:ALA:HA	1.67	0.77
1:G:163:ASP:HA	1:G:164:GLU:CB	2.15	0.76
1:G:216:TYR:O	1:G:219:ARG:HB3	1.86	0.76
1:C:266:ARG:NH1	1:C:269:GLN:NE2	2.33	0.76
1:F:123:LEU:H	1:F:123:LEU:CD2	1.99	0.76
1:D:121:GLN:NE2	1:D:130:ARG:CD	2.23	0.76
1:G:281:LEU:HD23	1:H:236:ARG:NH2	2.01	0.76
1:H:264:LEU:HD23	1:H:265:HIS:N	2.00	0.76
1:H:51:LYS:HB2	1:H:99:ARG:HG3	1.66	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:ALA:O	1:B:15:SER:HA	1.86	0.75
1:G:11:VAL:O	1:G:12:LEU:C	2.25	0.75
1:C:16:PHE:CD1	1:D:289:GLY:HA2	2.22	0.75
1:B:258:SER:O	1:B:262:HIS:HD2	1.69	0.75
1:E:76:THR:HG21	1:E:276:SER:N	2.02	0.74
1:C:268:LEU:CD2	1:D:250:HIS:CD2	2.71	0.73
1:F:76:THR:CG2	1:F:275:ALA:HA	2.18	0.73
1:E:76:THR:HG21	1:E:276:SER:H	1.52	0.73
1:C:49:ILE:HG23	1:D:56:GLN:HG2	1.70	0.73
1:F:212:GLU:OE2	1:F:212:GLU:C	2.26	0.73
1:H:287:THR:HB	1:H:288:HIS:HD2	1.53	0.73
1:C:28:ARG:NH1	1:C:235:GLU:HG2	2.04	0.73
1:B:43:PHE:CZ	1:B:249:LEU:HD13	2.23	0.73
1:F:296:TRP:N	1:F:296:TRP:CE3	2.49	0.73
1:H:76:THR:HG22	1:H:275:ALA:HA	1.69	0.73
1:C:14:GLY:O	1:C:18:GLU:HB2	1.89	0.73
1:A:290:PRO:C	1:A:292:MET:N	2.42	0.72
1:C:200:GLU:OE1	1:C:200:GLU:HA	1.90	0.72
1:E:235:GLU:OE1	1:E:235:GLU:CA	2.38	0.72
1:E:295:ASN:O	1:E:297:PRO:HD3	1.90	0.72
1:G:73:GLN:NE2	1:G:81:TRP:HE3	1.88	0.71
1:A:235:GLU:CG	1:A:238:ARG:NH2	2.51	0.71
1:D:121:GLN:HE22	1:D:130:ARG:HD2	1.50	0.71
1:F:27:GLN:HA	1:F:30:GLU:OE2	1.90	0.71
1:A:258:SER:O	1:A:262:HIS:CD2	2.43	0.71
1:E:96:LEU:O	1:E:96:LEU:HD12	1.90	0.70
1:G:85:PHE:O	1:G:89:GLU:HG2	1.91	0.70
1:G:140:GLN:HG2	1:G:220:TYR:HE1	1.55	0.70
1:A:99:ARG:NH1	1:A:103:HIS:CD2	2.58	0.70
1:F:258:SER:O	1:F:262:HIS:HD2	1.74	0.70
1:H:89:GLU:O	1:H:92:SER:HB3	1.91	0.70
1:A:270:GLN:HG2	2:A:347:HOH:O	1.90	0.70
1:C:285:ARG:CZ	1:D:225:GLU:OE2	2.40	0.70
1:C:28:ARG:HH11	1:C:235:GLU:HG2	1.57	0.70
1:E:40:VAL:O	1:E:44:GLN:HB2	1.92	0.70
1:A:268:LEU:HD23	1:B:250:HIS:CD2	2.26	0.70
1:D:24:ARG:HH11	1:D:24:ARG:HG2	1.56	0.70
1:H:216:TYR:O	1:H:218:PRO:HD2	1.92	0.69
1:E:264:LEU:HD12	1:E:265:HIS:N	2.07	0.69
1:F:20:GLY:O	1:F:23:ARG:HD2	1.92	0.69
1:A:24:ARG:HD2	1:B:288:HIS:ND1	2.08	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:235:GLU:HG3	1:F:239:LEU:HD22	1.75	0.69
1:C:141:LYS:O	1:C:142:PRO:C	2.30	0.69
1:A:76:THR:N	1:A:280:ASP:OD1	2.21	0.68
1:F:76:THR:HG21	1:F:276:SER:H	1.59	0.68
1:G:150:VAL:HG22	1:G:209:THR:HG23	1.76	0.68
1:G:115:ARG:O	1:G:119:HIS:CB	2.41	0.68
1:D:40:VAL:HG13	1:D:107:SER:HB3	1.74	0.68
1:H:235:GLU:OE1	1:H:238:ARG:NH1	2.27	0.68
1:B:121:GLN:HE22	1:B:130:ARG:HD2	1.59	0.68
1:F:212:GLU:OE2	1:F:212:GLU:CA	2.41	0.68
1:E:76:THR:N	1:E:280:ASP:OD1	2.26	0.68
1:G:266:ARG:NH1	1:G:269:GLN:HE21	1.90	0.68
1:E:264:LEU:HD12	1:E:264:LEU:C	2.14	0.67
1:F:260:LYS:NZ	1:F:260:LYS:CB	2.57	0.67
1:C:247:LEU:O	1:C:251:GLN:HG3	1.95	0.67
1:D:39:LEU:HD21	1:D:245:VAL:HG11	1.75	0.67
1:B:20:GLY:HA2	1:B:22:TYR:CE1	2.30	0.67
1:D:282:ARG:HH11	1:D:282:ARG:CG	2.08	0.67
1:C:281:LEU:HD21	1:D:236:ARG:HB2	1.77	0.66
1:E:272:ILE:CG2	1:F:247:LEU:HD13	2.25	0.66
1:C:228:PHE:CE2	1:C:232:GLN:NE2	2.63	0.66
1:F:120:ARG:HA	1:F:125:GLY:O	1.95	0.66
1:A:18:GLU:OE1	1:B:294:MET:SD	2.53	0.66
1:E:101:LYS:HD3	1:E:252:HIS:CE1	2.30	0.66
1:A:238:ARG:HH12	1:B:73:GLN:HE22	1.44	0.66
1:E:62:ARG:HG3	1:E:63:LYS:N	2.10	0.66
1:C:28:ARG:NH1	1:C:235:GLU:CG	2.58	0.65
1:H:287:THR:HB	1:H:288:HIS:CD2	2.30	0.65
1:A:292:MET:HG2	1:A:293:ALA:N	2.11	0.65
1:B:222:GLU:OE2	1:B:222:GLU:HA	1.96	0.65
1:A:260:LYS:O	1:A:263:GLU:HG2	1.96	0.65
1:A:26:VAL:O	1:A:29:VAL:HG23	1.96	0.65
1:E:76:THR:O	1:E:79:LYS:HB2	1.97	0.65
1:G:73:GLN:HE21	1:G:81:TRP:HE3	1.43	0.65
1:C:292:MET:H	1:C:292:MET:HE2	1.60	0.65
1:F:203:LYS:O	1:F:207:GLU:HG2	1.96	0.65
1:D:34:ARG:NH2	2:D:348:HOH:O	2.30	0.65
1:D:147:LEU:HD23	1:D:147:LEU:O	1.97	0.65
1:D:294:MET:O	1:D:294:MET:SD	2.53	0.65
1:F:204:THR:O	1:F:208:GLN:HG3	1.97	0.65
1:C:140:GLN:HG3	1:C:220:TYR:HE1	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:28:ARG:HH11	1:C:235:GLU:CG	2.10	0.65
1:C:14:GLY:C	1:C:18:GLU:HB2	2.17	0.64
1:C:266:ARG:HH11	1:C:269:GLN:HE21	1.43	0.64
1:A:99:ARG:HH12	1:A:103:HIS:CD2	2.15	0.64
1:H:248:THR:HG22	1:H:252:HIS:CE1	2.33	0.64
1:B:285:ARG:C	1:B:288:HIS:O	2.36	0.64
1:C:141:LYS:HD3	1:C:142:PRO:N	2.13	0.64
1:G:73:GLN:NE2	1:G:81:TRP:CE3	2.66	0.64
1:F:121:GLN:CD	1:F:130:ARG:HE	2.00	0.64
1:F:147:LEU:HD12	1:F:147:LEU:O	1.98	0.64
1:C:299:PHE:C	1:D:214:ASN:OD1	2.36	0.64
1:F:121:GLN:NE2	1:F:130:ARG:HE	1.94	0.63
1:F:213:LEU:HD12	1:F:213:LEU:C	2.17	0.63
1:F:225:GLU:OE1	1:F:229:GLU:OE2	2.16	0.63
1:D:76:THR:CG2	1:D:275:ALA:HA	2.28	0.63
1:G:6:ASP:HA	1:G:214:ASN:HD22	1.63	0.63
1:G:147:LEU:HD13	1:G:147:LEU:O	1.99	0.63
1:D:24:ARG:CG	1:D:24:ARG:NH1	2.57	0.63
1:B:73:GLN:OE1	1:B:77:LEU:HD23	2.00	0.62
1:C:232:GLN:HE21	1:D:285:ARG:HG3	1.64	0.62
1:G:254:ASP:OD1	1:G:256:SER:N	2.33	0.62
1:G:51:LYS:O	1:G:54:ALA:HB3	2.00	0.62
1:H:216:TYR:O	1:H:218:PRO:CD	2.48	0.62
1:F:94:LEU:HD11	1:F:260:LYS:HG2	1.82	0.61
1:G:49:ILE:HD13	1:H:56:GLN:HG2	1.80	0.61
1:G:20:GLY:O	1:G:23:ARG:HG3	2.00	0.61
1:H:143:TRP:CD1	1:H:143:TRP:C	2.74	0.61
1:F:123:LEU:CD2	1:F:123:LEU:N	2.61	0.61
1:C:266:ARG:NH1	1:C:269:GLN:HE22	1.97	0.61
1:G:139:ALA:O	1:G:142:PRO:HD2	2.01	0.61
1:H:20:GLY:O	1:H:23:ARG:HB2	2.00	0.61
1:C:17:TRP:CZ2	1:D:290:PRO:HB3	2.36	0.61
1:C:154:LYS:HG2	1:C:206:TYR:CE1	2.35	0.61
1:F:213:LEU:C	1:F:213:LEU:CD1	2.69	0.61
1:C:254:ASP:OD2	1:C:254:ASP:C	2.39	0.61
1:E:272:ILE:HG21	1:F:247:LEU:HD13	1.82	0.60
1:G:272:ILE:CG2	1:H:247:LEU:HD13	2.27	0.60
1:G:277:ASP:OD2	1:G:277:ASP:N	2.34	0.60
1:A:96:LEU:HD12	1:A:96:LEU:O	2.02	0.60
1:B:61:ALA:O	1:B:65:ARG:HB2	2.01	0.60
1:D:65:ARG:NE	2:D:352:HOH:O	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:140:GLN:HG3	1:C:220:TYR:CE1	2.37	0.59
1:D:235:GLU:OE2	1:D:238:ARG:HD3	2.01	0.59
1:A:157:TYR:CZ	1:A:203:LYS:HG3	2.37	0.59
1:B:202:MET:O	1:B:205:GLN:HG2	2.02	0.59
1:G:239:LEU:HD23	1:H:77:LEU:HD23	1.84	0.59
1:A:259:ASP:O	1:A:260:LYS:C	2.39	0.59
1:B:121:GLN:NE2	1:B:130:ARG:HD2	2.17	0.59
1:C:289:GLY:O	1:C:292:MET:CE	2.50	0.59
1:E:293:ALA:N	1:F:16:PHE:CB	2.64	0.59
1:B:235:GLU:HG3	1:B:239:LEU:HD22	1.84	0.59
1:C:31:ASP:OD1	1:C:34:ARG:NH2	2.35	0.59
1:C:264:LEU:HD12	1:C:265:HIS:N	2.17	0.59
1:H:99:ARG:C	1:H:99:ARG:HD3	2.23	0.59
1:E:292:MET:O	1:E:294:MET:N	2.36	0.59
1:B:42:CYS:O	1:B:42:CYS:SG	2.60	0.59
1:B:222:GLU:OE2	1:B:222:GLU:CA	2.50	0.59
1:B:283:TRP:CZ2	1:B:287:THR:HG21	2.37	0.58
1:C:269:GLN:O	1:C:273:GLU:HG3	2.03	0.58
1:D:99:ARG:HD3	1:D:99:ARG:C	2.23	0.58
1:F:92:SER:OG	1:F:93:GLU:N	2.36	0.58
1:G:120:ARG:O	1:G:121:GLN:C	2.39	0.58
1:C:40:VAL:O	1:C:44:GLN:HB2	2.03	0.58
1:D:39:LEU:CD2	1:D:245:VAL:HG11	2.33	0.58
1:D:51:LYS:HB2	1:D:99:ARG:HG3	1.84	0.58
1:E:96:LEU:O	1:E:96:LEU:CD1	2.51	0.58
1:H:206:TYR:CZ	1:H:210:LEU:HD12	2.38	0.58
1:E:258:SER:HB3	1:E:261:PHE:CB	2.34	0.58
1:H:204:THR:HG22	1:H:208:GLN:HE21	1.69	0.58
1:D:217:THR:O	1:D:221:MET:HG3	2.04	0.58
1:G:46:ARG:NE	1:G:50:GLU:OE2	2.31	0.58
1:C:235:GLU:CD	1:C:238:ARG:HH21	2.07	0.58
1:G:20:GLY:O	1:G:23:ARG:CG	2.52	0.57
1:G:141:LYS:HB3	1:G:142:PRO:HD3	1.84	0.57
1:C:157:TYR:CE1	1:C:203:LYS:HB2	2.38	0.57
1:A:103:HIS:CG	1:A:103:HIS:O	2.56	0.57
1:E:106:ASP:OD1	1:E:252:HIS:CE1	2.58	0.57
1:E:163:ASP:HB3	1:E:164:GLU:OE2	2.04	0.57
1:G:80:ALA:O	1:G:83:ALA:HB3	2.04	0.57
1:H:205:GLN:O	1:H:209:THR:HG23	2.05	0.57
1:A:28:ARG:NH2	1:A:232:GLN:OE1	2.38	0.57
1:A:40:VAL:O	1:A:44:GLN:HB2	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:272:ILE:HG21	1:D:247:LEU:CD1	2.35	0.57
1:G:260:LYS:O	1:G:264:LEU:HB3	2.03	0.57
1:A:76:THR:HG21	1:A:275:ALA:CA	2.26	0.57
1:E:106:ASP:OD1	1:E:252:HIS:ND1	2.38	0.57
1:G:77:LEU:HD22	1:H:239:LEU:HD12	1.86	0.57
1:A:140:GLN:HG3	1:A:220:TYR:CE1	2.40	0.57
1:E:275:ALA:O	1:F:243:LYS:NZ	2.36	0.57
1:D:20:GLY:O	1:D:23:ARG:HB2	2.04	0.56
1:C:71:GLY:HA2	2:D:348:HOH:O	2.05	0.56
1:D:298:GLN:O	1:D:299:PHE:CB	2.51	0.56
1:A:49:ILE:HG23	1:B:56:GLN:HG2	1.88	0.56
1:D:24:ARG:NH1	1:D:24:ARG:HG3	2.20	0.56
1:G:6:ASP:CA	1:G:214:ASN:HD22	2.16	0.56
1:H:39:LEU:HD22	1:H:242:PHE:CE1	2.40	0.56
1:E:73:GLN:NE2	1:E:81:TRP:HE3	1.99	0.56
1:E:293:ALA:N	1:F:16:PHE:HB3	2.21	0.56
1:B:54:ALA:O	1:B:92:SER:HB2	2.05	0.56
1:G:68:VAL:HG21	1:G:81:TRP:CE2	2.40	0.56
1:G:72:PRO:HG2	1:H:35:LEU:HD21	1.88	0.56
1:D:202:MET:HA	1:D:202:MET:CE	2.36	0.56
1:G:35:LEU:HD11	1:H:72:PRO:HD2	1.86	0.56
1:C:28:ARG:NH1	1:C:235:GLU:CB	2.69	0.56
1:F:212:GLU:OE2	1:F:212:GLU:HA	2.06	0.56
1:G:161:ARG:O	1:G:164:GLU:CB	2.54	0.56
1:C:272:ILE:HG21	1:D:247:LEU:HD13	1.89	0.56
1:B:203:LYS:HA	1:B:206:TYR:HB3	1.88	0.55
1:D:76:THR:HG21	1:D:275:ALA:HA	1.87	0.55
1:A:272:ILE:HG21	1:B:247:LEU:HD23	1.88	0.55
1:D:121:GLN:CD	1:D:130:ARG:HD3	2.21	0.55
1:B:277:ASP:OD2	1:B:278:GLU:N	2.40	0.55
1:A:51:LYS:O	1:A:55:GLN:HG2	2.07	0.55
1:D:287:THR:HB	1:D:288:HIS:HD2	1.71	0.55
1:E:15:SER:HA	1:F:292:MET:SD	2.47	0.55
1:E:35:LEU:HD23	1:F:73:GLN:HE21	1.71	0.55
1:F:23:ARG:NH2	1:F:133:GLU:OE1	2.39	0.55
1:C:147:LEU:HD12	1:C:147:LEU:O	2.07	0.55
1:E:263:GLU:HG3	1:E:264:LEU:N	2.22	0.55
1:E:281:LEU:HD23	1:F:236:ARG:NH2	2.22	0.55
1:E:298:GLN:H	1:E:298:GLN:HE21	1.55	0.55
1:F:121:GLN:OE1	1:F:130:ARG:NE	2.40	0.55
1:G:268:LEU:HD23	1:H:250:HIS:CD2	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:94:LEU:HG	1:H:260:LYS:HD3	1.88	0.54
1:F:143:TRP:CD1	1:F:143:TRP:C	2.79	0.54
1:C:275:ALA:O	1:D:243:LYS:NZ	2.41	0.54
1:F:34:ARG:NH2	2:F:345:HOH:O	2.41	0.54
1:A:140:GLN:HG3	1:A:220:TYR:HE1	1.73	0.54
1:B:206:TYR:CD2	1:B:207:GLU:HG3	2.43	0.54
1:E:278:GLU:OE2	1:E:278:GLU:HA	2.07	0.54
1:C:153:SER:HB2	1:C:209:THR:HG21	1.89	0.54
1:H:121:GLN:HE22	1:H:130:ARG:CG	2.20	0.54
1:A:35:LEU:HD13	1:B:73:GLN:HE21	1.73	0.53
1:A:96:LEU:O	1:A:96:LEU:CD1	2.56	0.53
1:G:140:GLN:OE1	1:G:144:LEU:HD11	2.07	0.53
1:C:150:VAL:HG22	1:C:209:THR:HG23	1.89	0.53
1:H:261:PHE:O	1:H:264:LEU:HD22	2.08	0.53
1:B:16:PHE:CG	1:B:16:PHE:O	2.61	0.53
1:H:89:GLU:O	1:H:93:GLU:HG3	2.08	0.53
1:F:30:GLU:OE1	1:F:129:SER:CB	2.57	0.53
1:B:121:GLN:OE1	1:B:130:ARG:HD2	2.08	0.53
1:E:150:VAL:HG21	1:E:213:LEU:HG	1.91	0.53
1:H:24:ARG:NH2	2:H:346:HOH:O	2.41	0.53
1:A:247:LEU:HG	1:B:272:ILE:HG21	1.90	0.53
1:A:94:LEU:O	1:A:98:VAL:HG23	2.08	0.53
1:A:298:GLN:O	1:A:299:PHE:CB	2.56	0.53
1:G:140:GLN:HG2	1:G:220:TYR:CE1	2.41	0.53
1:A:157:TYR:CE1	1:A:203:LYS:HG3	2.44	0.52
1:C:20:GLY:HA2	1:C:22:TYR:CE1	2.43	0.52
1:G:7:ALA:N	1:G:214:ASN:ND2	2.57	0.52
1:B:205:GLN:HG3	1:B:206:TYR:N	2.23	0.52
1:F:51:LYS:HB2	1:F:99:ARG:HG3	1.90	0.52
1:D:205:GLN:HG3	1:D:206:TYR:N	2.23	0.52
1:E:108:GLU:OE2	1:E:111:ARG:HD2	2.10	0.52
1:F:260:LYS:HB2	1:F:260:LYS:HZ2	1.68	0.52
1:A:278:GLU:HA	1:A:278:GLU:OE2	2.09	0.52
1:D:143:TRP:HZ3	1:D:217:THR:HG1	1.57	0.52
1:C:232:GLN:NE2	1:D:285:ARG:HG3	2.24	0.52
1:A:256:SER:O	1:A:262:HIS:HE1	1.93	0.52
1:C:206:TYR:O	1:C:209:THR:HG22	2.09	0.52
1:D:102:LEU:N	1:D:102:LEU:HD12	2.24	0.52
1:H:143:TRP:CD1	1:H:144:LEU:N	2.78	0.52
1:A:106:ASP:OD2	1:A:252:HIS:ND1	2.41	0.52
1:E:125:GLY:H	1:E:130:ARG:HH21	1.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:47:ALA:HB1	1:H:99:ARG:HG2	1.93	0.51
1:H:261:PHE:O	1:H:264:LEU:HD23	2.09	0.51
1:H:264:LEU:HD21	1:H:265:HIS:CD2	2.45	0.51
1:D:217:THR:HB	1:D:218:PRO:HD3	1.93	0.51
1:E:298:GLN:NE2	1:E:298:GLN:O	2.43	0.51
1:F:277:ASP:OD2	1:F:278:GLU:N	2.43	0.51
1:A:55:GLN:O	1:A:58:ALA:HB3	2.10	0.51
1:B:223:ASP:O	1:B:226:GLN:HB2	2.09	0.51
1:E:272:ILE:HG22	1:F:247:LEU:HD13	1.91	0.51
1:C:285:ARG:NH1	1:D:225:GLU:OE2	2.44	0.51
1:A:290:PRO:O	1:A:292:MET:N	2.44	0.51
1:A:133:GLU:O	1:A:133:GLU:HG3	2.11	0.51
1:C:51:LYS:O	1:C:54:ALA:HB3	2.11	0.51
1:F:228:PHE:HE2	1:F:232:GLN:HE21	1.58	0.51
1:E:65:ARG:CZ	1:E:82:HIS:CG	2.93	0.51
1:B:260:LYS:O	1:B:264:LEU:HB3	2.11	0.51
1:C:299:PHE:CA	1:D:214:ASN:OD1	2.59	0.51
1:D:164:GLU:CG	1:D:196:THR:N	2.74	0.51
1:H:235:GLU:OE2	1:H:235:GLU:HA	2.11	0.51
1:B:43:PHE:CE2	1:B:249:LEU:HD13	2.47	0.50
1:D:64:TRP:HA	1:D:67:ALA:HB3	1.92	0.50
1:H:238:ARG:O	1:H:242:PHE:HD2	1.95	0.50
1:D:47:ALA:HB1	1:D:99:ARG:HG2	1.93	0.50
1:E:238:ARG:HH12	1:F:73:GLN:NE2	2.09	0.50
1:E:250:HIS:ND1	1:F:268:LEU:HD23	2.25	0.50
1:G:11:VAL:O	1:G:12:LEU:O	2.28	0.50
1:H:216:TYR:O	1:H:218:PRO:N	2.44	0.50
1:A:254:ASP:OD2	1:A:256:SER:N	2.44	0.50
1:G:100:GLU:OE2	1:G:100:GLU:HA	2.11	0.50
1:A:95:HIS:CE1	1:A:255:LEU:HD11	2.46	0.50
1:B:235:GLU:HG3	1:B:235:GLU:O	2.10	0.50
1:E:258:SER:HB3	1:E:261:PHE:HB3	1.93	0.50
1:C:272:ILE:CG2	1:D:247:LEU:HD13	2.41	0.50
1:E:145:LYS:O	1:E:149:GLU:HG3	2.11	0.50
1:A:263:GLU:O	1:A:267:ASP:OD2	2.29	0.50
1:D:202:MET:HA	1:D:202:MET:HE2	1.94	0.50
1:H:277:ASP:OD2	1:H:278:GLU:N	2.44	0.50
1:A:277:ASP:OD2	1:A:278:GLU:N	2.43	0.50
1:G:258:SER:O	1:G:262:HIS:HD2	1.95	0.50
1:E:15:SER:O	1:E:18:GLU:HB2	2.12	0.50
1:G:6:ASP:HB3	1:G:214:ASN:ND2	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:254:ASP:OD2	1:C:256:SER:OG	2.27	0.50
1:B:24:ARG:NH2	2:B:342:HOH:O	2.45	0.49
1:D:276:SER:HG	1:D:279:GLU:HB3	1.77	0.49
1:H:85:PHE:O	1:H:88:ALA:HB3	2.12	0.49
1:B:15:SER:N	2:B:345:HOH:O	2.44	0.49
1:G:26:VAL:O	1:G:29:VAL:HG23	2.12	0.49
1:G:140:GLN:O	1:G:144:LEU:HD12	2.11	0.49
1:A:99:ARG:O	1:A:103:HIS:HB3	2.12	0.49
1:A:141:LYS:HB3	1:A:142:PRO:HD3	1.94	0.49
1:D:50:GLU:OE2	1:D:95:HIS:ND1	2.35	0.49
1:A:256:SER:HB3	1:B:265:HIS:CD2	2.46	0.49
1:B:264:LEU:C	1:B:264:LEU:HD23	2.31	0.49
1:E:258:SER:HB3	1:E:261:PHE:HB2	1.93	0.49
1:E:293:ALA:N	1:F:16:PHE:CA	2.75	0.49
1:B:164:GLU:HG3	1:B:196:THR:HA	1.94	0.49
1:D:89:GLU:O	1:D:93:GLU:HG3	2.13	0.49
1:F:61:ALA:O	1:F:65:ARG:HB2	2.11	0.49
1:F:96:LEU:HD12	1:F:96:LEU:O	2.11	0.49
1:C:227:ALA:O	1:C:228:PHE:C	2.51	0.49
1:D:151:GLU:OE2	1:D:151:GLU:HA	2.13	0.49
1:D:277:ASP:O	1:D:280:ASP:N	2.45	0.49
1:E:76:THR:CG2	1:E:276:SER:H	2.22	0.49
1:F:297:PRO:O	1:F:298:GLN:HG2	2.13	0.49
1:A:284:TRP:CD1	1:B:28:ARG:NH1	2.81	0.49
1:B:200:GLU:O	1:B:203:LYS:HD3	2.12	0.49
1:F:108:GLU:O	1:F:109:ARG:C	2.51	0.49
1:G:258:SER:O	1:G:262:HIS:CD2	2.66	0.49
1:B:147:LEU:HA	1:B:213:LEU:CD1	2.43	0.49
1:D:90:ARG:NH1	1:D:260:LYS:HE2	2.28	0.49
1:H:35:LEU:O	1:H:36:CYS:C	2.51	0.49
1:B:242:PHE:O	1:B:243:LYS:C	2.52	0.48
1:H:121:GLN:CD	1:H:130:ARG:HD2	2.31	0.48
1:E:65:ARG:CZ	1:E:82:HIS:CB	2.89	0.48
1:G:7:ALA:H	1:G:214:ASN:ND2	2.11	0.48
1:G:264:LEU:C	1:G:264:LEU:HD23	2.33	0.48
1:B:64:TRP:HB3	1:B:85:PHE:CZ	2.48	0.48
1:F:255:LEU:O	1:F:258:SER:HB3	2.13	0.48
1:H:259:ASP:O	1:H:260:LYS:C	2.52	0.48
1:B:157:TYR:HB2	1:B:202:MET:HB3	1.94	0.48
1:H:219:ARG:NH1	1:H:219:ARG:HG3	2.27	0.48
1:A:217:THR:O	1:A:221:MET:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:72:PRO:HG3	1:F:34:ARG:NH1	2.28	0.48
1:C:292:MET:H	1:C:292:MET:CE	2.27	0.48
1:E:77:LEU:HD22	1:F:239:LEU:HD12	1.94	0.48
1:G:49:ILE:HG23	1:H:56:GLN:HG2	1.95	0.48
1:A:275:ALA:O	1:B:243:LYS:CE	2.61	0.48
1:F:46:ARG:NH2	1:F:50:GLU:OE1	2.37	0.48
1:E:28:ARG:CZ	1:E:235:GLU:HG2	2.44	0.48
1:E:266:ARG:O	1:E:269:GLN:HB3	2.14	0.48
1:F:151:GLU:OE2	1:F:151:GLU:CA	2.54	0.48
1:H:266:ARG:O	1:H:269:GLN:HB3	2.14	0.48
1:C:25:THR:O	1:C:28:ARG:HB3	2.13	0.48
1:F:121:GLN:HE22	1:F:130:ARG:HE	1.62	0.48
1:G:136:PHE:HD1	1:G:224:MET:CE	2.26	0.48
1:G:136:PHE:HD1	1:G:224:MET:HE2	1.79	0.48
1:A:270:GLN:HA	1:A:273:GLU:HG3	1.96	0.47
1:B:219:ARG:O	1:B:222:GLU:HB3	2.14	0.47
1:A:83:ALA:HB1	1:A:268:LEU:HD12	1.95	0.47
1:A:268:LEU:O	1:A:269:GLN:C	2.53	0.47
1:E:108:GLU:OE2	1:E:111:ARG:CD	2.62	0.47
1:G:264:LEU:HD23	1:G:265:HIS:N	2.29	0.47
1:D:40:VAL:O	1:D:44:GLN:HG3	2.15	0.47
1:F:43:PHE:CD1	1:F:249:LEU:HG	2.50	0.47
1:F:212:GLU:OE2	1:F:213:LEU:N	2.48	0.47
1:G:283:TRP:O	1:G:284:TRP:C	2.53	0.47
1:C:217:THR:O	1:C:221:MET:HG3	2.15	0.47
1:C:292:MET:HB2	1:D:16:PHE:H	1.79	0.47
1:D:119:HIS:HB2	1:D:127:ARG:HG2	1.95	0.47
1:C:289:GLY:C	1:C:291:GLY:H	2.18	0.47
1:F:64:TRP:HB3	1:F:85:PHE:CZ	2.49	0.47
1:F:80:ALA:O	1:F:83:ALA:HB3	2.15	0.47
1:H:254:ASP:OD1	1:H:254:ASP:C	2.52	0.47
1:B:16:PHE:O	1:B:16:PHE:CD1	2.68	0.47
1:C:284:TRP:O	1:C:285:ARG:C	2.51	0.47
1:G:272:ILE:HG21	1:H:247:LEU:CD1	2.30	0.47
1:C:289:GLY:O	1:C:292:MET:HE2	2.14	0.47
1:E:236:ARG:HB2	1:F:281:LEU:HD11	1.97	0.47
1:E:258:SER:C	1:E:262:HIS:CD2	2.89	0.47
1:A:256:SER:O	1:A:262:HIS:CE1	2.68	0.47
1:A:269:GLN:O	1:A:273:GLU:HG2	2.15	0.47
1:A:249:LEU:HD23	1:A:249:LEU:HA	1.83	0.46
1:E:140:GLN:HG3	1:E:220:TYR:HE1	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:LEU:HD12	1:A:265:HIS:N	2.30	0.46
1:H:228:PHE:CE2	1:H:232:GLN:NE2	2.83	0.46
1:D:76:THR:N	1:D:280:ASP:OD1	2.36	0.46
1:E:76:THR:HG21	1:E:275:ALA:C	2.34	0.46
1:G:49:ILE:HD13	1:H:56:GLN:CG	2.46	0.46
1:A:46:ARG:HD2	1:A:46:ARG:O	2.14	0.46
1:E:40:VAL:HG13	1:E:107:SER:HB3	1.98	0.46
1:H:228:PHE:CE2	1:H:232:GLN:HG3	2.51	0.46
1:A:163:ASP:N	1:A:163:ASP:OD1	2.48	0.46
1:A:289:GLY:O	1:A:292:MET:HB3	2.16	0.46
1:D:20:GLY:H	1:D:140:GLN:HE22	1.64	0.46
1:E:165:LYS:HD2	1:E:165:LYS:N	2.31	0.46
1:E:43:PHE:CD2	1:E:249:LEU:HD13	2.51	0.46
1:G:278:GLU:O	1:G:279:GLU:C	2.53	0.46
1:C:228:PHE:HE2	1:D:285:ARG:HG3	1.80	0.46
1:H:39:LEU:HD22	1:H:242:PHE:HE1	1.80	0.46
1:E:203:LYS:O	1:E:207:GLU:HB2	2.16	0.46
1:G:20:GLY:HA2	1:G:22:TYR:CD1	2.50	0.45
1:G:206:TYR:O	1:G:209:THR:HG22	2.16	0.45
1:G:254:ASP:OD1	1:G:254:ASP:C	2.54	0.45
1:F:50:GLU:OE2	1:F:95:HIS:ND1	2.45	0.45
1:A:63:LYS:HG2	1:A:64:TRP:N	2.31	0.45
1:B:235:GLU:OE2	1:B:238:ARG:HD3	2.16	0.45
1:G:120:ARG:CA	1:G:127:ARG:H	2.29	0.45
1:D:24:ARG:HH11	1:D:24:ARG:HG3	1.71	0.45
1:E:94:LEU:O	1:E:98:VAL:HG23	2.16	0.45
1:F:99:ARG:HD3	1:F:99:ARG:C	2.36	0.45
1:H:50:GLU:OE2	1:H:95:HIS:ND1	2.48	0.45
1:E:43:PHE:CG	1:E:249:LEU:HD13	2.51	0.45
1:C:235:GLU:CD	1:C:238:ARG:HE	2.19	0.45
1:D:201:LYS:HD2	1:D:202:MET:HE1	1.99	0.45
1:D:223:ASP:O	1:D:226:GLN:HB2	2.16	0.45
1:E:101:LYS:HB3	1:E:252:HIS:ND1	2.32	0.45
1:F:213:LEU:HD12	1:F:214:ASN:N	2.31	0.45
1:G:268:LEU:CD2	1:H:250:HIS:CD2	2.99	0.45
1:B:76:THR:HA	1:B:79:LYS:HG3	1.99	0.45
1:C:86:THR:HA	1:C:89:GLU:OE2	2.17	0.45
1:D:90:ARG:HH11	1:D:260:LYS:HE2	1.81	0.45
1:G:281:LEU:HD23	1:H:236:ARG:HH21	1.81	0.45
1:B:164:GLU:OE1	1:B:196:THR:HA	2.17	0.45
1:B:198:GLU:O	1:B:201:LYS:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:196:THR:CG2	1:D:196:THR:CA	2.85	0.45
1:F:228:PHE:CE2	1:F:232:GLN:NE2	2.83	0.45
1:E:140:GLN:HG3	1:E:220:TYR:CE1	2.52	0.45
1:B:258:SER:O	1:B:262:HIS:CD2	2.60	0.44
1:C:17:TRP:HZ2	1:D:290:PRO:HB3	1.82	0.44
1:E:72:PRO:HD2	1:F:35:LEU:HD11	1.99	0.44
1:E:141:LYS:HB3	1:E:142:PRO:HD3	1.99	0.44
1:A:247:LEU:HG	1:B:272:ILE:CG2	2.47	0.44
1:A:267:ASP:OD2	1:A:267:ASP:N	2.51	0.44
1:F:121:GLN:HG2	1:F:125:GLY:HA3	1.98	0.44
1:B:141:LYS:O	1:B:144:LEU:N	2.48	0.44
1:C:144:LEU:HD12	1:C:144:LEU:HA	1.74	0.44
1:D:106:ASP:O	1:D:110:VAL:HG23	2.17	0.44
1:D:255:LEU:O	1:D:258:SER:HB3	2.18	0.44
1:E:83:ALA:HB1	1:E:268:LEU:HD12	2.00	0.44
1:E:146:ARG:HG3	1:E:146:ARG:HH11	1.82	0.44
1:E:62:ARG:CG	1:E:63:LYS:N	2.78	0.44
1:E:84:PHE:HA	1:E:268:LEU:CD1	2.48	0.44
1:G:56:GLN:OE1	1:H:49:ILE:HG12	2.17	0.44
1:C:17:TRP:HZ3	1:C:221:MET:HA	1.82	0.44
1:E:269:GLN:HA	1:E:269:GLN:OE1	2.17	0.44
1:F:204:THR:O	1:F:208:GLN:CG	2.64	0.44
1:B:120:ARG:HA	1:B:125:GLY:O	2.18	0.44
1:C:216:TYR:O	1:C:219:ARG:HB3	2.18	0.44
1:A:272:ILE:HG21	1:B:247:LEU:CD2	2.47	0.44
1:D:201:LYS:HD2	1:D:202:MET:CE	2.48	0.44
1:F:106:ASP:OD1	1:F:106:ASP:N	2.50	0.44
1:B:228:PHE:CE2	1:B:232:GLN:NE2	2.86	0.43
1:B:255:LEU:O	1:B:258:SER:HB3	2.18	0.43
1:C:150:VAL:HA	1:C:209:THR:HG23	2.00	0.43
1:E:75:GLY:HA3	1:E:280:ASP:OD1	2.18	0.43
1:G:249:LEU:HA	1:G:249:LEU:HD23	1.79	0.43
1:F:22:TYR:O	1:F:23:ARG:C	2.57	0.43
1:G:275:ALA:O	1:H:243:LYS:CE	2.67	0.43
1:H:276:SER:OG	1:H:279:GLU:HB2	2.19	0.43
1:C:292:MET:CE	1:C:292:MET:N	2.81	0.43
1:C:298:GLN:O	1:C:299:PHE:CB	2.67	0.43
1:F:140:GLN:NE2	1:F:144:LEU:HD11	2.34	0.43
1:B:101:LYS:HD3	1:B:252:HIS:CD2	2.54	0.43
1:C:150:VAL:HA	1:C:209:THR:CG2	2.48	0.43
1:C:210:LEU:HD22	1:C:214:ASN:OD1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:277:ASP:OD1	1:C:277:ASP:N	2.45	0.43
1:D:99:ARG:HD3	1:D:100:GLU:N	2.34	0.43
1:E:96:LEU:CD1	1:E:96:LEU:C	2.87	0.43
1:E:264:LEU:C	1:E:264:LEU:CD1	2.84	0.43
1:B:40:VAL:HG13	1:B:107:SER:HB3	2.01	0.43
1:C:281:LEU:HD12	1:C:281:LEU:HA	1.80	0.43
1:G:291:GLY:O	1:H:15:SER:OG	2.36	0.43
1:F:104:GLY:HA3	1:F:105:PRO:HD3	1.89	0.43
1:G:65:ARG:HH22	1:G:82:HIS:HB3	1.76	0.43
1:G:239:LEU:HD23	1:H:77:LEU:CD2	2.47	0.43
1:E:101:LYS:O	1:E:105:PRO:HD2	2.18	0.43
1:E:160:ALA:HA	1:E:163:ASP:HB2	2.01	0.43
1:B:203:LYS:HE3	1:B:203:LYS:C	2.40	0.43
1:D:65:ARG:O	1:D:66:GLY:C	2.56	0.43
1:D:276:SER:OG	1:D:279:GLU:CB	2.67	0.43
1:E:285:ARG:NH1	1:F:225:GLU:OE2	2.48	0.43
1:F:295:ASN:N	1:F:296:TRP:CE3	2.87	0.43
1:G:73:GLN:HG3	1:G:78:GLU:HB2	2.01	0.43
1:H:219:ARG:HH11	1:H:219:ARG:CG	2.32	0.43
1:B:248:THR:CG2	1:B:252:HIS:CE1	3.01	0.43
1:D:90:ARG:NH1	1:D:260:LYS:CE	2.82	0.43
1:A:65:ARG:O	1:A:69:GLU:HB3	2.19	0.42
1:C:35:LEU:CD1	1:D:72:PRO:HD2	2.30	0.42
1:E:16:PHE:CD2	1:E:16:PHE:O	2.72	0.42
1:H:81:TRP:O	1:H:82:HIS:C	2.57	0.42
1:F:258:SER:O	1:F:262:HIS:CD2	2.64	0.42
1:H:121:GLN:OE1	1:H:130:ARG:HD2	2.19	0.42
1:E:65:ARG:O	1:E:69:GLU:HB3	2.19	0.42
1:E:269:GLN:OE1	1:E:269:GLN:CA	2.67	0.42
1:H:64:TRP:HA	1:H:67:ALA:HB3	2.01	0.42
1:C:100:GLU:OE2	1:C:100:GLU:HA	2.18	0.42
1:E:24:ARG:HD2	1:E:24:ARG:HA	1.67	0.42
1:F:33:HIS:HB2	1:F:118:PHE:CD2	2.54	0.42
1:E:260:LYS:HA	1:E:263:GLU:HG2	2.00	0.42
1:H:77:LEU:HD12	1:H:77:LEU:HA	1.74	0.42
1:E:99:ARG:HG3	1:E:100:GLU:N	2.34	0.42
1:A:258:SER:HB3	1:A:261:PHE:CB	2.50	0.42
1:D:39:LEU:HD21	1:D:245:VAL:CG1	2.45	0.42
1:G:61:ALA:O	1:G:65:ARG:HB3	2.19	0.42
1:A:17:TRP:HB2	1:B:294:MET:HG2	2.01	0.42
1:D:64:TRP:HA	1:D:67:ALA:CB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:284:TRP:O	1:E:285:ARG:C	2.57	0.42
1:H:28:ARG:CZ	1:H:235:GLU:HG2	2.50	0.42
1:E:21:ASN:C	1:E:23:ARG:H	2.22	0.42
1:E:47:ALA:O	1:E:50:GLU:HB2	2.20	0.42
1:G:247:LEU:O	1:G:251:GLN:HG3	2.20	0.42
1:H:14:GLY:HA2	1:H:17:TRP:HD1	1.84	0.42
1:A:103:HIS:CD2	1:A:103:HIS:O	2.73	0.42
1:C:261:PHE:CE2	1:D:256:SER:HB3	2.55	0.42
1:E:73:GLN:NE2	1:E:81:TRP:CE3	2.84	0.42
1:E:251:GLN:HE21	1:E:251:GLN:HB3	1.72	0.42
1:H:106:ASP:O	1:H:110:VAL:HG23	2.19	0.42
1:C:260:LYS:HA	1:C:263:GLU:HG2	2.00	0.41
1:C:281:LEU:HD23	1:D:236:ARG:NH2	2.35	0.41
1:D:119:HIS:CD2	1:D:127:ARG:NH1	2.88	0.41
1:D:212:GLU:HA	1:D:215:ARG:HD2	2.02	0.41
1:E:254:ASP:OD2	1:E:256:SER:OG	2.32	0.41
1:G:120:ARG:O	1:G:122:VAL:N	2.53	0.41
1:C:266:ARG:HD3	1:C:266:ARG:HA	1.88	0.41
1:D:255:LEU:HA	1:D:255:LEU:HD12	1.68	0.41
1:E:147:LEU:HD12	1:E:147:LEU:O	2.20	0.41
1:E:225:GLU:OE2	1:F:285:ARG:NH2	2.36	0.41
1:C:215:ARG:O	1:C:218:PRO:HD2	2.21	0.41
1:E:298:GLN:HE21	1:E:298:GLN:N	2.16	0.41
1:B:115:ARG:HA	1:B:120:ARG:HH22	1.85	0.41
1:C:268:LEU:HD21	1:D:250:HIS:CD2	2.55	0.41
1:C:278:GLU:O	1:C:279:GLU:C	2.59	0.41
1:C:292:MET:HB3	1:D:15:SER:HA	2.03	0.41
1:E:16:PHE:CD2	1:E:16:PHE:C	2.93	0.41
1:E:20:GLY:HA2	1:E:22:TYR:CE1	2.55	0.41
1:H:64:TRP:HB3	1:H:85:PHE:CZ	2.55	0.41
1:H:121:GLN:NE2	1:H:130:ARG:CD	2.59	0.41
1:E:35:LEU:HD12	1:E:35:LEU:HA	1.87	0.41
1:D:120:ARG:CD	1:D:120:ARG:N	2.59	0.41
1:G:153:SER:HB2	1:G:209:THR:HG21	2.01	0.41
1:A:104:GLY:HA3	1:A:105:PRO:HD3	1.93	0.41
1:B:79:LYS:H	1:B:79:LYS:HG2	1.48	0.41
1:B:121:GLN:CD	1:B:130:ARG:HD2	2.41	0.41
1:C:36:CYS:O	1:C:40:VAL:HG23	2.20	0.41
1:C:84:PHE:CE2	1:D:246:LEU:HD22	2.55	0.41
1:D:77:LEU:HD23	1:D:77:LEU:HA	1.45	0.41
1:D:81:TRP:O	1:D:84:PHE:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:120:ARG:CA	1:D:125:GLY:O	2.53	0.41
1:D:202:MET:HA	1:D:205:GLN:HG2	2.03	0.41
1:G:6:ASP:CA	1:G:214:ASN:ND2	2.82	0.41
1:H:219:ARG:NH1	1:H:219:ARG:CG	2.84	0.41
1:H:276:SER:O	1:H:277:ASP:C	2.58	0.41
1:A:269:GLN:O	1:A:272:ILE:HB	2.20	0.41
1:C:82:HIS:O	1:C:83:ALA:C	2.58	0.41
1:E:104:GLY:HA3	1:E:105:PRO:HD3	1.88	0.41
1:A:51:LYS:HB2	1:A:99:ARG:HG2	2.02	0.41
1:A:236:ARG:HB2	1:B:281:LEU:HD11	2.02	0.41
1:B:150:VAL:HG21	1:B:210:LEU:HD22	2.03	0.41
1:C:203:LYS:O	1:C:206:TYR:HB3	2.21	0.41
1:D:28:ARG:CZ	1:D:235:GLU:HG2	2.50	0.41
1:E:96:LEU:HD12	1:E:96:LEU:C	2.40	0.41
1:E:294:MET:CA	1:F:17:TRP:HD1	2.33	0.41
1:F:124:GLY:HA3	1:F:125:GLY:HA3	1.66	0.41
1:F:260:LYS:CB	1:F:260:LYS:HZ2	2.28	0.41
1:G:266:ARG:NH1	1:G:269:GLN:NE2	2.64	0.41
1:A:240:LEU:HD21	1:B:277:ASP:OD1	2.21	0.41
1:C:247:LEU:HD13	1:C:247:LEU:HA	1.95	0.41
1:D:38:ASP:O	1:D:39:LEU:C	2.57	0.41
1:D:228:PHE:CE2	1:D:232:GLN:HG3	2.56	0.41
1:E:238:ARG:HH12	1:F:73:GLN:HE22	1.68	0.41
1:G:140:GLN:O	1:G:141:LYS:C	2.60	0.41
1:B:202:MET:O	1:B:205:GLN:CG	2.68	0.40
1:C:55:GLN:O	1:C:58:ALA:HB3	2.20	0.40
1:A:102:LEU:O	1:A:107:SER:HB2	2.21	0.40
1:D:43:PHE:CE1	1:D:249:LEU:HG	2.56	0.40
1:D:202:MET:CE	1:D:202:MET:CA	2.99	0.40
1:E:21:ASN:C	1:E:21:ASN:OD1	2.60	0.40
1:E:101:LYS:HB3	1:E:252:HIS:HD1	1.85	0.40
1:E:254:ASP:OD2	1:E:254:ASP:C	2.59	0.40
1:G:104:GLY:O	1:G:108:GLU:HB3	2.21	0.40
1:H:203:LYS:O	1:H:207:GLU:HG2	2.21	0.40
1:A:273:GLU:HG2	1:A:273:GLU:H	1.67	0.40
1:B:228:PHE:HE2	1:B:232:GLN:NE2	2.19	0.40
1:B:264:LEU:HD23	1:B:265:HIS:N	2.36	0.40
1:D:258:SER:HB3	1:D:261:PHE:CB	2.52	0.40
1:E:249:LEU:HA	1:E:249:LEU:HD23	1.73	0.40
1:F:25:THR:O	1:F:25:THR:CG2	2.70	0.40
1:H:141:LYS:C	1:H:141:LYS:HE2	2.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:ARG:HA	1:A:65:ARG:CZ	2.51	0.40
1:A:76:THR:HG21	1:A:276:SER:H	1.86	0.40
1:E:279:GLU:HA	1:E:282:ARG:CZ	2.52	0.40
1:D:276:SER:OG	1:D:279:GLU:HB3	2.21	0.40
1:F:126:PHE:O	1:F:130:ARG:HB2	2.21	0.40
1:F:240:LEU:O	1:F:241:PHE:C	2.60	0.40
1:F:254:ASP:OD1	1:F:254:ASP:C	2.59	0.40
1:G:22:TYR:O	1:G:26:VAL:HG23	2.21	0.40
1:G:97:GLU:O	1:G:98:VAL:C	2.58	0.40
1:G:236:ARG:HB2	1:H:281:LEU:HD11	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	243/347 (70%)	229 (94%)	10 (4%)	4 (2%)	9	37
1	B	253/347 (73%)	236 (93%)	14 (6%)	3 (1%)	13	44
1	C	251/347 (72%)	231 (92%)	20 (8%)	0	100	100
1	D	249/347 (72%)	230 (92%)	17 (7%)	2 (1%)	19	54
1	E	249/347 (72%)	232 (93%)	16 (6%)	1 (0%)	34	69
1	F	247/347 (71%)	224 (91%)	21 (8%)	2 (1%)	19	54
1	G	250/347 (72%)	222 (89%)	25 (10%)	3 (1%)	13	44
1	H	241/347 (70%)	224 (93%)	14 (6%)	3 (1%)	13	44
All	All	1983/2776 (71%)	1828 (92%)	137 (7%)	18 (1%)	17	52

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	213	LEU
1	F	297	PRO
1	B	290	PRO
1	D	71	GLY
1	H	71	GLY
1	H	104	GLY
1	D	124	GLY
1	G	12	LEU
1	H	290	PRO
1	A	83	ALA
1	B	104	GLY
1	B	291	GLY
1	G	10	GLU
1	G	11	VAL
1	A	72	PRO
1	A	291	GLY
1	E	290	PRO
1	A	290	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	201/294 (68%)	173 (86%)	28 (14%)	3 15
1	B	210/294 (71%)	177 (84%)	33 (16%)	2 11
1	C	197/294 (67%)	154 (78%)	43 (22%)	1 4
1	D	205/294 (70%)	172 (84%)	33 (16%)	2 10
1	E	196/294 (67%)	157 (80%)	39 (20%)	1 5
1	F	193/294 (66%)	157 (81%)	36 (19%)	1 7
1	G	182/294 (62%)	143 (79%)	39 (21%)	1 4
1	H	186/294 (63%)	159 (86%)	27 (14%)	3 13
All	All	1570/2352 (67%)	1292 (82%)	278 (18%)	2 8

All (278) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ARG
1	A	29	VAL
1	A	51	LYS
1	A	55	GLN
1	A	73	GLN
1	A	96	LEU
1	A	99	ARG
1	A	120	ARG
1	A	123	LEU
1	A	129	SER
1	A	130	ARG
1	A	148	LYS
1	A	155	LYS
1	A	163	ASP
1	A	204	THR
1	A	217	THR
1	A	224	MET
1	A	230	SER
1	A	246	LEU
1	A	248	THR
1	A	251	GLN
1	A	255	LEU
1	A	256	SER
1	A	257	SER
1	A	266	ARG
1	A	267	ASP
1	A	269	GLN
1	A	271	SER
1	B	15	SER
1	B	21	ASN
1	B	23	ARG
1	B	30	GLU
1	B	35	LEU
1	B	56	GLN
1	B	62	ARG
1	B	70	LYS
1	B	89	GLU
1	B	120	ARG
1	B	123	LEU
1	B	127	ARG
1	B	129	SER
1	B	133	GLU
1	B	140	GLN

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Mol	Chain	Res	Type
1	B	148	LYS
1	B	150	VAL
1	B	158	HIS
1	B	201	LYS
1	B	202	MET
1	B	203	LYS
1	B	210	LEU
1	B	224	MET
1	B	230	SER
1	B	238	ARG
1	B	239	LEU
1	B	258	SER
1	B	260	LYS
1	B	264	LEU
1	B	270	GLN
1	B	276	SER
1	B	279	GLU
1	B	298	GLN
1	C	23	ARG
1	C	30	GLU
1	C	35	LEU
1	C	50	GLU
1	C	55	GLN
1	C	56	GLN
1	C	57	LEU
1	C	73	GLN
1	C	76	THR
1	C	79	LYS
1	C	90	ARG
1	C	93	GLU
1	C	99	ARG
1	C	114	GLN
1	C	130	ARG
1	C	137	ARG
1	C	144	LEU
1	C	145	LYS
1	C	147	LEU
1	C	148	LYS
1	C	154	LYS
1	C	159	THR
1	C	200	GLU
1	C	202	MET

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Mol	Chain	Res	Type
1	C	204	THR
1	C	207	GLU
1	C	209	THR
1	C	210	LEU
1	C	212	GLU
1	C	217	THR
1	C	219	ARG
1	C	224	MET
1	C	244	ASP
1	C	246	LEU
1	C	247	LEU
1	C	257	SER
1	C	259	ASP
1	C	266	ARG
1	C	271	SER
1	C	277	ASP
1	C	279	GLU
1	C	281	LEU
1	C	292	MET
1	D	21	ASN
1	D	23	ARG
1	D	24	ARG
1	D	35	LEU
1	D	56	GLN
1	D	62	ARG
1	D	109	ARG
1	D	120	ARG
1	D	133	GLU
1	D	143	TRP
1	D	148	LYS
1	D	158	HIS
1	D	197	LYS
1	D	201	LYS
1	D	202	MET
1	D	210	LEU
1	D	221	MET
1	D	224	MET
1	D	238	ARG
1	D	239	LEU
1	D	247	LEU
1	D	248	THR
1	D	249	LEU

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Mol	Chain	Res	Type
1	D	255	LEU
1	D	257	SER
1	D	266	ARG
1	D	269	GLN
1	D	278	GLU
1	D	282	ARG
1	D	285	ARG
1	D	286	SER
1	D	287	THR
1	D	294	MET
1	E	18	GLU
1	E	30	GLU
1	E	34	ARG
1	E	35	LEU
1	E	41	SER
1	E	55	GLN
1	E	86	THR
1	E	90	ARG
1	E	96	LEU
1	E	99	ARG
1	E	107	SER
1	E	115	ARG
1	E	130	ARG
1	E	144	LEU
1	E	161	ARG
1	E	164	GLU
1	E	165	LYS
1	E	208	GLN
1	E	212	GLU
1	E	215	ARG
1	E	217	THR
1	E	219	ARG
1	E	224	MET
1	E	235	GLU
1	E	237	GLN
1	E	246	LEU
1	E	247	LEU
1	E	257	SER
1	E	263	GLU
1	E	264	LEU
1	E	266	ARG
1	E	270	GLN

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Mol	Chain	Res	Type
1	E	271	SER
1	E	276	SER
1	E	281	LEU
1	E	287	THR
1	E	290	PRO
1	E	295	ASN
1	E	298	GLN
1	F	21	ASN
1	F	23	ARG
1	F	28	ARG
1	F	34	ARG
1	F	35	LEU
1	F	48	ARG
1	F	51	LYS
1	F	57	LEU
1	F	73	GLN
1	F	76	THR
1	F	89	GLU
1	F	109	ARG
1	F	122	VAL
1	F	123	LEU
1	F	130	ARG
1	F	133	GLU
1	F	143	TRP
1	F	148	LYS
1	F	151	GLU
1	F	158	HIS
1	F	210	LEU
1	F	212	GLU
1	F	213	LEU
1	F	215	ARG
1	F	219	ARG
1	F	224	MET
1	F	230	SER
1	F	239	LEU
1	F	247	LEU
1	F	249	LEU
1	F	258	SER
1	F	260	LYS
1	F	278	GLU
1	F	282	ARG
1	F	296	TRP

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Mol	Chain	Res	Type
1	F	298	GLN
1	G	18	GLU
1	G	24	ARG
1	G	30	GLU
1	G	34	ARG
1	G	35	LEU
1	G	55	GLN
1	G	57	LEU
1	G	62	ARG
1	G	65	ARG
1	G	76	THR
1	G	89	GLU
1	G	90	ARG
1	G	96	LEU
1	G	99	ARG
1	G	114	GLN
1	G	121	GLN
1	G	123	LEU
1	G	141	LYS
1	G	144	LEU
1	G	147	LEU
1	G	153	SER
1	G	209	THR
1	G	210	LEU
1	G	212	GLU
1	G	213	LEU
1	G	226	GLN
1	G	230	SER
1	G	246	LEU
1	G	247	LEU
1	G	255	LEU
1	G	260	LYS
1	G	264	LEU
1	G	266	ARG
1	G	267	ASP
1	G	269	GLN
1	G	271	SER
1	G	279	GLU
1	G	281	LEU
1	G	287	THR
1	H	16	PHE
1	H	23	ARG

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Mol	Chain	Res	Type
1	H	30	GLU
1	H	35	LEU
1	H	41	SER
1	H	56	GLN
1	H	57	LEU
1	H	62	ARG
1	H	73	GLN
1	H	89	GLU
1	H	109	ARG
1	H	127	ARG
1	H	141	LYS
1	H	143	TRP
1	H	147	LEU
1	H	216	TYR
1	H	219	ARG
1	H	230	SER
1	H	238	ARG
1	H	239	LEU
1	H	247	LEU
1	H	248	THR
1	H	249	LEU
1	H	258	SER
1	H	264	LEU
1	H	286	SER
1	H	287	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	HIS
1	A	44	GLN
1	A	82	HIS
1	A	103	HIS
1	A	208	GLN
1	A	251	GLN
1	A	262	HIS
1	A	270	GLN
1	B	55	GLN
1	B	73	GLN
1	B	82	HIS
1	B	208	GLN
1	B	226	GLN

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Mol	Chain	Res	Type
1	B	250	HIS
1	B	262	HIS
1	B	265	HIS
1	C	73	GLN
1	C	226	GLN
1	C	232	GLN
1	C	251	GLN
1	C	252	HIS
1	C	265	HIS
1	C	269	GLN
1	C	270	GLN
1	C	288	HIS
1	D	55	GLN
1	D	119	HIS
1	D	121	GLN
1	D	140	GLN
1	D	205	GLN
1	D	250	HIS
1	D	251	GLN
1	D	265	HIS
1	D	288	HIS
1	E	73	GLN
1	E	226	GLN
1	E	237	GLN
1	E	251	GLN
1	E	262	HIS
1	E	298	GLN
1	F	56	GLN
1	F	73	GLN
1	F	82	HIS
1	F	140	GLN
1	F	205	GLN
1	F	226	GLN
1	F	237	GLN
1	F	250	HIS
1	F	262	HIS
1	F	288	HIS
1	F	298	GLN
1	G	44	GLN
1	G	82	HIS
1	G	214	ASN
1	G	250	HIS

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Mol	Chain	Res	Type
1	G	251	GLN
1	G	265	HIS
1	G	269	GLN
1	H	55	GLN
1	H	82	HIS
1	H	119	HIS
1	H	121	GLN
1	H	140	GLN
1	H	208	GLN
1	H	237	GLN
1	H	250	HIS
1	H	265	HIS
1	H	270	GLN
1	H	288	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	250/347 (72%)	0.36	5 (2%) 65 44	37, 61, 103, 129	0
1	B	257/347 (74%)	0.41	8 (3%) 49 26	25, 55, 120, 137	0
1	C	257/347 (74%)	0.38	3 (1%) 79 61	42, 59, 97, 112	0
1	D	255/347 (73%)	0.38	5 (1%) 65 44	34, 54, 120, 135	0
1	E	255/347 (73%)	0.40	8 (3%) 49 26	39, 59, 108, 127	0
1	F	255/347 (73%)	0.46	10 (3%) 39 20	32, 55, 101, 114	0
1	G	254/347 (73%)	0.34	6 (2%) 59 37	41, 59, 83, 98	0
1	H	247/347 (71%)	0.39	2 (0%) 86 72	35, 53, 89, 102	0
All	All	2030/2776 (73%)	0.39	47 (2%) 60 39	25, 57, 103, 137	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	292	MET	7.4
1	C	293	ALA	6.4
1	F	293	ALA	5.8
1	E	291	GLY	5.0
1	E	166	THR	4.9
1	B	291	GLY	4.8
1	F	291	GLY	4.8
1	B	293	ALA	4.6
1	A	19	ALA	4.1
1	D	159	THR	3.9
1	B	159	THR	3.6
1	F	169	THR	3.6
1	A	292	MET	3.5
1	D	19	ALA	3.3
1	G	291	GLY	3.1
1	E	158	HIS	3.0

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Mol	Chain	Res	Type	RSRZ
1	F	292	MET	2.8
1	E	162	LYS	2.8
1	E	164	GLU	2.8
1	F	16	PHE	2.6
1	B	19	ALA	2.6
1	D	17	TRP	2.5
1	F	295	ASN	2.5
1	G	204	THR	2.5
1	H	14	GLY	2.4
1	E	157	TYR	2.4
1	D	160	ALA	2.4
1	C	81	TRP	2.4
1	F	143	TRP	2.3
1	A	162	LYS	2.3
1	B	16	PHE	2.3
1	C	292	MET	2.3
1	F	166	THR	2.3
1	D	16	PHE	2.3
1	G	81	TRP	2.2
1	E	249	LEU	2.2
1	H	291	GLY	2.2
1	B	220	TYR	2.1
1	A	132	ALA	2.1
1	G	114	GLN	2.1
1	G	253	LEU	2.1
1	F	217	THR	2.0
1	A	249	LEU	2.0
1	G	239	LEU	2.0
1	B	143	TRP	2.0
1	F	242	PHE	2.0
1	E	165	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides 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.