



Full wwPDB X-ray Structure Validation Report ⓘ

May 27, 2020 – 04:06 am BST

PDB ID : 5J7U
Title : Faustovirus major capsid protein
Authors : Klose, T.; Rossmann, M.G.
Deposited on : 2016-04-06
Resolution : 2.44 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

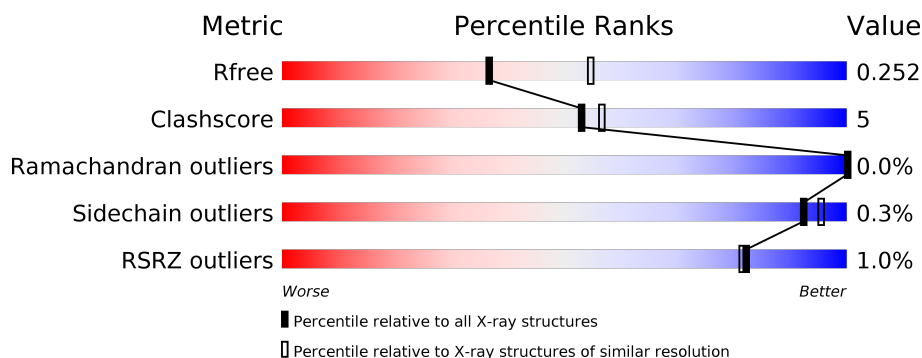
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.44 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.


















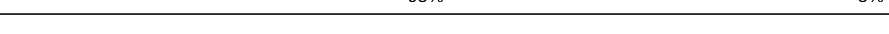

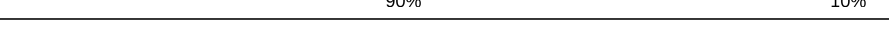
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1564 (2.46-2.42)
Clashscore	141614	1631 (2.46-2.42)
Ramachandran outliers	138981	1617 (2.46-2.42)
Sidechain outliers	138945	1617 (2.46-2.42)
RSRZ outliers	127900	1547 (2.46-2.42)

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 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	645	
1	B	645	
1	C	645	
1	D	645	
1	E	645	
1	F	645	

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Mol	Chain	Length	Quality of chain
1	G	645	
1	H	645	
1	I	645	
1	J	645	
1	K	645	
1	L	645	
2	M	21	
2	N	21	
2	O	21	
2	P	21	
2	Q	21	
2	R	21	
2	S	21	
2	T	21	
2	U	21	
2	V	21	
2	W	21	
2	X	21	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 61035 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 major capsid protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	609	Total	C	N	O	S	0	0	0
			4785	3060	803	908	14			
1	B	616	Total	C	N	O	S	0	0	0
			4837	3092	812	919	14			
1	C	616	Total	C	N	O	S	0	0	0
			4842	3098	812	918	14			
1	D	609	Total	C	N	O	S	0	0	0
			4785	3060	803	908	14			
1	E	616	Total	C	N	O	S	0	0	0
			4841	3097	812	918	14			
1	F	610	Total	C	N	O	S	0	0	0
			4793	3064	804	911	14			
1	G	611	Total	C	N	O	S	0	0	0
			4799	3067	805	913	14			
1	H	615	Total	C	N	O	S	0	0	0
			4831	3089	811	917	14			
1	I	616	Total	C	N	O	S	0	0	0
			4842	3098	812	918	14			
1	J	610	Total	C	N	O	S	0	0	0
			4793	3064	804	911	14			
1	K	614	Total	C	N	O	S	0	0	0
			4823	3083	810	916	14			
1	L	610	Total	C	N	O	S	0	0	0
			4793	3064	804	911	14			

- Molecule 2 is a protein called unknown.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	M	21	Total	C	N	O	0	0	0
			105	63	21	21			
2	N	21	Total	C	N	O	0	0	0
			105	63	21	21			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	O	21	Total	C	N	O	0	0	0
			105	63	21	21			
2	P	21	Total	C	N	O	0	0	0
			105	63	21	21			
2	Q	21	Total	C	N	O	0	0	0
			105	63	21	21			
2	R	19	Total	C	N	O	0	0	0
			95	57	19	19			
2	S	21	Total	C	N	O	0	0	0
			105	63	21	21			
2	T	21	Total	C	N	O	0	0	0
			105	63	21	21			
2	U	21	Total	C	N	O	0	0	0
			105	63	21	21			
2	V	21	Total	C	N	O	0	0	0
			105	63	21	21			
2	W	21	Total	C	N	O	0	0	0
			105	63	21	21			
2	X	19	Total	C	N	O	0	0	0
			95	57	19	19			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	173	Total	O	0	0
			173	173		
3	B	170	Total	O	0	0
			170	170		
3	C	164	Total	O	0	0
			164	164		
3	D	191	Total	O	0	0
			191	191		
3	E	168	Total	O	0	0
			168	168		
3	F	172	Total	O	0	0
			172	172		
3	N	2	Total	O	0	0
			2	2		
3	O	2	Total	O	0	0
			2	2		
3	P	5	Total	O	0	0
			5	5		

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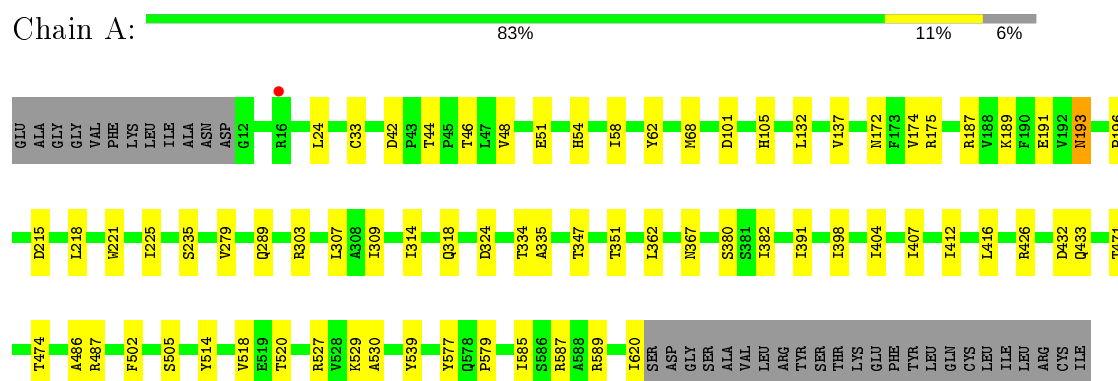
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	Q	2	Total 2	O 2	0	0
3	R	2	Total 2	O 2	0	0
3	G	176	Total 176	O 176	0	0
3	H	165	Total 165	O 165	0	0
3	I	133	Total 133	O 133	0	0
3	J	163	Total 163	O 163	0	0
3	K	156	Total 156	O 156	0	0
3	L	171	Total 171	O 171	0	0
3	S	1	Total 1	O 1	0	0
3	U	7	Total 7	O 7	0	0
3	V	3	Total 3	O 3	0	0
3	W	2	Total 2	O 2	0	0
3	X	3	Total 3	O 3	0	0

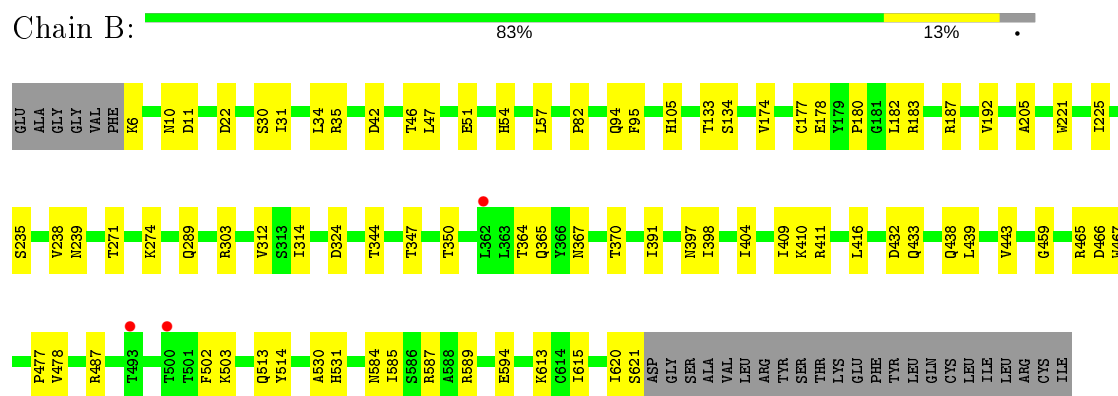
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

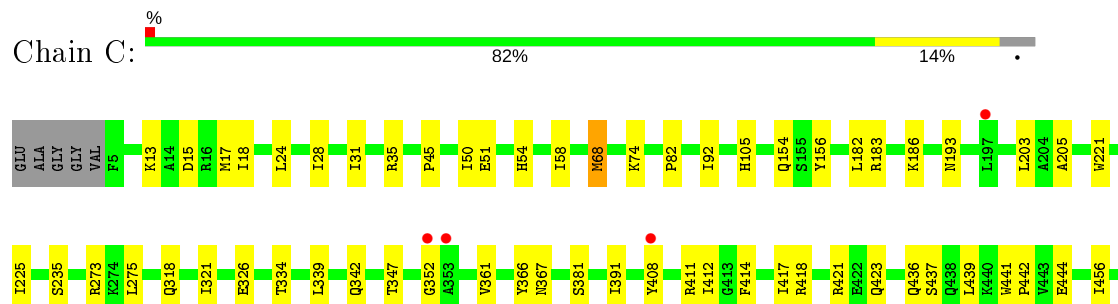
- Molecule 1: major capsid protein

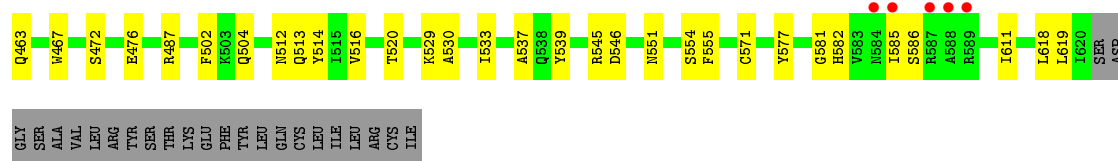


- Molecule 1: major capsid protein

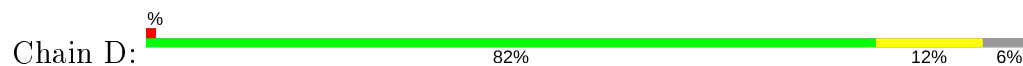


- Molecule 1: major capsid protein

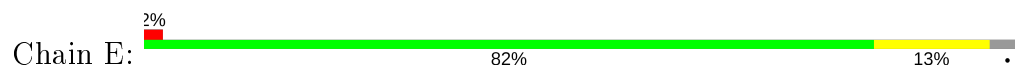




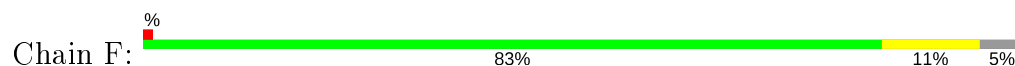
- Molecule 1: major capsid protein

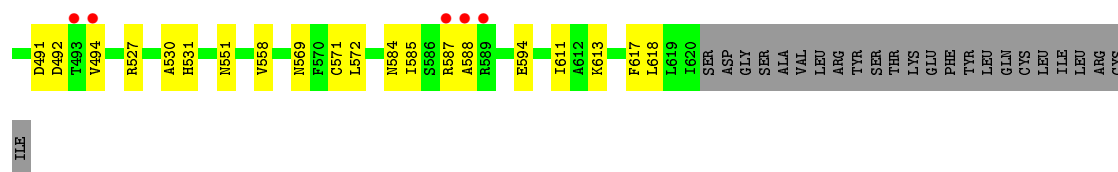


- Molecule 1: major capsid protein



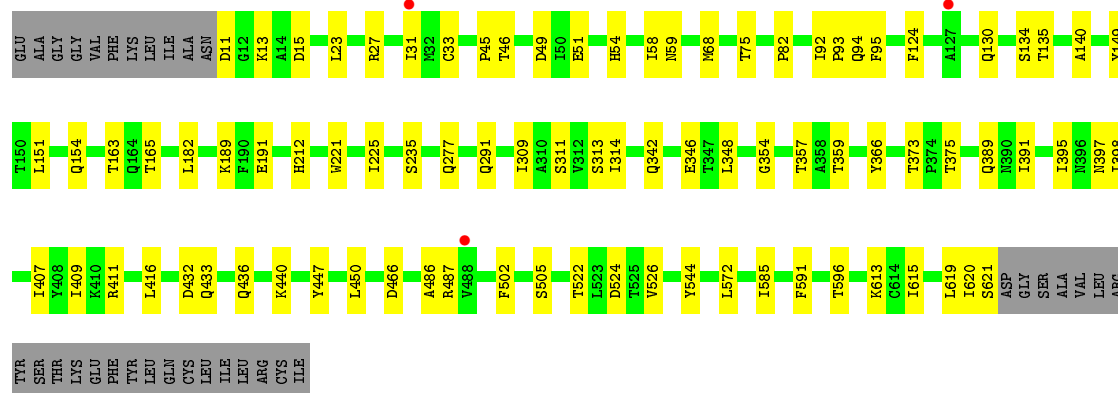
- Molecule 1: major capsid protein





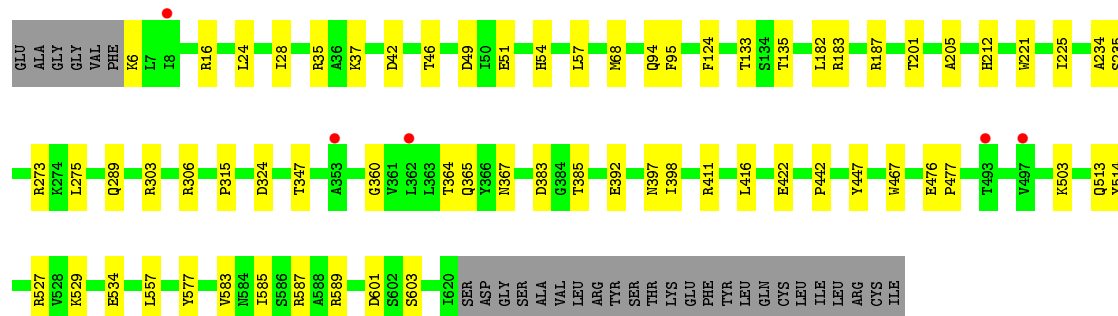
- Molecule 1: major capsid protein

Chain G: 81% 13% 5%



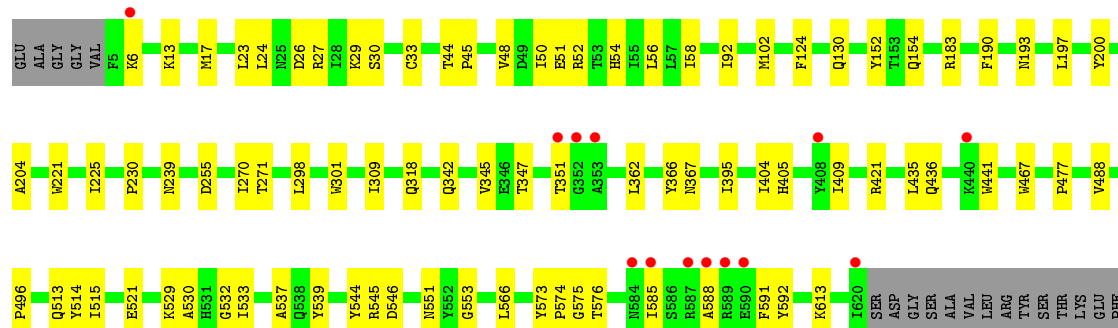
- Molecule 1: major capsid protein

Chain H: 85% 10% 5%




- Molecule 1: major capsid protein

Chain I: 82% 13% 5%



TYR
LEU
GLN
CYS
LEU
LEU
ILE
LEU
ARG
CYS
ILE

- Molecule 1: major capsid protein


Chain J:  84% 11% 5%

GLU
ALA
GLY
GLY
VAL
PHE
LYS
LEU
ILE
ASN
D11
I18
L24
R27
T44
D49
I50
E51
R52
I53
H54
I55
I58
P82
H105
S112
F124
Q130
Y152
P180
G181
L182
K186
R187
V188
K189
F190
E191
P196
L197
A205
I206

K210
R223
L224
I225
S235
D255
G258
T259
A260
V261
A272
R273
K274
L275
T288
D304
P305
R306
P315
Q318
D324
I325
E326
V345
I348
I349
T350
A353
T357
A358
T359
I391
I398
I404
I407
F414
L439
P442
V443

L448
E476
I490
T501
Y514
K529
R540
A541
Q542
H582
Y583
N584
R587
E594
F599
N604
L608
L618
L619
I620
GLY
SER
ALA
VAL
LEU
ARG
TYR
SER
THR
LYS
PHE
TYR
LEU
GLN
CYS
ILE
ARG
CYS
ILE

- Molecule 1: major capsid protein

Chain K:  82% 13% 5%


GLU
ALA
GLY
GLY
VAL
PHE
K6
L7
I8
D15
L24
I31
R35
D42
P43
T44
T46
D49
I50
E51
H54
I55
I56
L57
K63
R76
G80
Q89
F95
G96
D101
L108
F124
I125
G126
Q130
T133
T135
S139

Y149
V157
N158
M172
F173
V174
P180
R183
R187
V188
K189
F190
E191
V192
N193
D215
T219
G220
M221
R222
L224
I225
G226
I270
Q277
V278
T284
Q289
L292
N293
M294
P295
V296
L298
R303
T322
D324
T347
T357
T359

C360
V361
L362
N367
S380
N390
N397
I398
F399
R411
T415
R418
Q436
E444
I467
N512
Q513
Y514
N584
I585
S586
R587
A588
R589
E590
F591
M616
F617
L618
L619
I619
SER
ASP
GLY
SER
ALA
VAL
LEU
ARG
TYR
SER
THR
LYS
GLU
PHE
TYR
LEU

GLN
CYS
LEU
ILE
LEU
ARG
CYS
CYS
ILE

- Molecule 1: major capsid protein

Chain L:  82% 12% 5%

GLU
ALA
GLY
GLY
VAL
PHE
LYS
LEU
ILE
ASN
D11
G12
K13
A14
R16
L24
R27
I28
C33
P45
V48
D49
I50
E51
R52
I53
H54
I58
M58
T75
I92
P93
D101
M102
H105
A110
L121
I125
T135
S136
V137
T141

Y152
T153
Q154
T163
E178
R183
L203
K210
W221
I225
S235
V238
K274
P285
R303
D304
E326
A335
Q342
T343
T347
N367
I391
I395
I404
K410
R411
I412
T415
V434
Q438
L439
P442
V443

R485
P486
P487
Y485
A486
R487
D492
T493
F502
K503
Q504
H531
G532
I533
R545
P546
Y547
D562
K563
N584
I585
S586
R587
E590
L608
I609
L615
L618
L619
I620
SER
ASP
GLY
SER
SER
VAL
LEU
ARG
TYR
SER
THR
LYS
GLU
PHE
TYR
LEU
GLN
CYS
LEU

ILE
LEU
ARG
CYS
CYS
ILE

- Molecule 2: unknown

Chain M:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: unknown

Chain N:  95% 5%



- Molecule 2: unknown

Chain O:  100%


There are no outlier residues recorded for this chain.

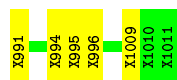
- Molecule 2: unknown

Chain P:  95% 5%



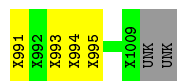
- Molecule 2: unknown

Chain Q:  76% 24%




- Molecule 2: unknown

Chain R:  71% 19% 10%



- Molecule 2: unknown

Chain S:  86% 14%



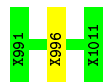
- Molecule 2: unknown

Chain T:  100%


There are no outlier residues recorded for this chain.

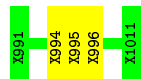
- Molecule 2: unknown

Chain U:  95% 5%



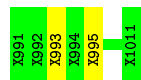
- Molecule 2: unknown

Chain V:  86% 14%



- Molecule 2: unknown

Chain W:  90% 10%



- Molecule 2: unknown

Chain X:  67% 24% 10%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	86.38Å 390.83Å 130.14Å 90.00° 91.66° 90.00°	Depositor
Resolution (Å)	72.92 – 2.44 72.92 – 2.44	Depositor EDS
% Data completeness (in resolution range)	99.6 (72.92-2.44) 99.8 (72.92-2.44)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 2.45Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.205 , 0.252 0.205 , 0.252	Depositor DCC
R_{free} test set	15720 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	39.2	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 42.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.039 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	61035	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.29 % 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 1.1691e-04. 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	0.26	0/4901	0.48	0/6697
1	B	0.26	0/4953	0.48	0/6767
1	C	0.27	0/4959	0.49	0/6775
1	D	0.26	0/4901	0.47	0/6697
1	E	0.26	0/4958	0.48	0/6774
1	F	0.26	0/4909	0.48	0/6708
1	G	0.27	0/4915	0.48	0/6716
1	H	0.26	0/4947	0.47	0/6759
1	I	0.26	0/4959	0.47	0/6775
1	J	0.26	0/4909	0.47	0/6708
1	K	0.27	0/4939	0.48	0/6748
1	L	0.26	0/4909	0.48	0/6708
All	All	0.26	0/59159	0.48	0/80832

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	4785	0	4711	72	0
1	B	4837	0	4766	61	0
1	C	4842	0	4770	63	0
1	D	4785	0	4711	65	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	4841	0	4768	72	0
1	F	4793	0	4715	57	0
1	G	4799	0	4720	56	0
1	H	4831	0	4761	47	0
1	I	4842	0	4770	59	0
1	J	4793	0	4715	55	0
1	K	4823	0	4750	61	0
1	L	4793	0	4715	57	0
2	M	105	0	24	0	0
2	N	105	0	24	1	0
2	O	105	0	24	0	0
2	P	105	0	24	1	0
2	Q	105	0	24	4	0
2	R	95	0	21	4	0
2	S	105	0	24	3	0
2	T	105	0	24	0	0
2	U	105	0	25	1	0
2	V	105	0	25	3	0
2	W	105	0	24	1	0
2	X	95	0	22	5	0
3	A	173	0	0	3	0
3	B	170	0	0	5	0
3	C	164	0	0	2	0
3	D	191	0	0	4	0
3	E	168	0	0	3	0
3	F	172	0	0	3	0
3	G	176	0	0	5	0
3	H	165	0	0	7	0
3	I	133	0	0	3	0
3	J	163	0	0	4	0
3	K	156	0	0	4	0
3	L	171	0	0	5	0
3	N	2	0	0	1	0
3	O	2	0	0	0	0
3	P	5	0	0	0	0
3	Q	2	0	0	1	0
3	R	2	0	0	2	0
3	S	1	0	0	1	0
3	U	7	0	0	0	0
3	V	3	0	0	0	0
3	W	2	0	0	1	0
3	X	3	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	61035	0	57157	628	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 5.

All (628) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:527:ARG:HH12	1:A:529:LYS:CE	1.25	1.44
1:D:62:TYR:CE1	1:E:416:LEU:CD1	2.02	1.43
1:D:62:TYR:CE1	1:E:416:LEU:HD13	1.53	1.40
1:A:527:ARG:NH1	1:A:529:LYS:HE3	1.36	1.36
1:A:351:THR:OG1	1:A:362:LEU:HD22	1.14	1.30
1:I:318:GLN:CD	3:I:701:HOH:O	1.73	1.26
1:D:62:TYR:CZ	1:E:416:LEU:HD11	1.74	1.22
1:I:318:GLN:NE2	3:I:701:HOH:O	1.71	1.19
1:A:351:THR:OG1	1:A:362:LEU:CD2	2.02	1.07
1:D:62:TYR:CD1	1:E:416:LEU:HD13	1.97	0.99
1:D:62:TYR:CZ	1:E:416:LEU:CD1	2.42	0.91
1:A:527:ARG:HH12	1:A:529:LYS:HE3	0.74	0.91
1:C:436:GLN:HB3	1:C:439:LEU:HD23	1.50	0.91
1:D:404:ILE:HD11	1:F:24:LEU:HD21	1.54	0.88
1:D:273:ARG:HE	1:E:284:THR:HG22	1.37	0.87
1:A:527:ARG:NH1	1:A:529:LYS:CE	2.08	0.83
1:K:35:ARG:NH1	1:K:42:ASP:O	2.13	0.81
1:E:582:HIS:NE2	1:F:15:ASP:OD1	2.13	0.80
1:D:62:TYR:HE1	1:E:416:LEU:CD1	1.90	0.80
1:F:35:ARG:NH2	1:F:42:ASP:O	2.17	0.77
1:D:44:THR:O	1:E:411:ARG:NH2	2.18	0.76
1:B:187:ARG:NH1	1:B:324:ASP:OD2	2.18	0.76
1:G:75:THR:HG21	1:G:93:PRO:HG2	1.67	0.76
1:J:273:ARG:HE	1:K:284:THR:HG22	1.51	0.75
1:E:500:THR:O	1:E:503:LYS:NZ	2.21	0.74
1:A:46:THR:HG22	1:A:48:VAL:H	1.52	0.74
1:K:180:PRO:HB2	1:K:294:MET:HE1	1.69	0.74
1:J:112:SER:HB3	1:J:288:THR:HG22	1.69	0.73
1:I:102:MET:HE3	1:I:298:LEU:HD12	1.71	0.73
1:B:433:GLN:HG2	1:B:594:GLU:HG2	1.70	0.73
1:D:62:TYR:OH	1:E:416:LEU:HD11	1.89	0.72
1:A:175:ARG:HH11	1:A:335:ALA:HB2	1.53	0.72
1:H:303:ARG:NH1	1:I:551:ASN:OD1	2.21	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:527:ARG:HH12	1:A:529:LYS:CD	2.02	0.72
1:G:357:THR:HG23	1:G:359:THR:H	1.55	0.72
1:I:26:ASP:HA	1:I:29:LYS:HG2	1.71	0.72
1:D:58:ILE:HD11	1:E:398:ILE:HG21	1.72	0.72
1:J:540:ARG:NH1	1:J:542:GLN:OE1	2.24	0.71
1:F:133:THR:HG23	1:F:135:THR:H	1.56	0.71
1:B:178:GLU:HG3	1:B:465:ARG:HA	1.73	0.71
1:G:189:LYS:NZ	1:G:191:GLU:OE2	2.22	0.71
1:I:33:CYS:SG	3:I:793:HOH:O	2.48	0.70
1:G:13:LYS:NZ	2:S:1009:UNK:O	2.24	0.70
2:S:991:UNK:N	3:S:1101:HOH:O	2.25	0.70
1:A:527:ARG:HH12	1:A:529:LYS:HE2	1.50	0.70
1:F:16:ARG:NH2	3:F:705:HOH:O	2.25	0.69
1:H:35:ARG:NH2	1:H:42:ASP:O	2.25	0.69
1:B:585:ILE:HG22	1:B:589:ARG:HE	1.58	0.69
1:H:306:ARG:NH1	3:H:705:HOH:O	2.24	0.69
1:L:33:CYS:SG	3:L:834:HOH:O	2.49	0.69
1:K:357:THR:OG1	1:K:359:THR:HG22	1.93	0.68
1:D:35:ARG:NH2	1:D:42:ASP:O	2.23	0.68
1:K:133:THR:HG23	1:K:135:THR:H	1.57	0.68
1:F:81:ASN:OD1	1:F:81:ASN:O	2.11	0.68
1:E:357:THR:OG1	1:E:359:THR:HG22	1.92	0.68
1:J:58:ILE:HD11	1:K:398:ILE:HG21	1.75	0.68
1:E:31:ILE:HG21	1:E:45:PRO:HB3	1.76	0.68
1:L:531:HIS:CD2	1:L:587:ARG:HA	2.29	0.68
1:E:44:THR:O	1:F:411:ARG:NH2	2.22	0.67
1:A:33:CYS:SG	3:A:850:HOH:O	2.51	0.67
1:A:539:TYR:HE1	1:C:74:LYS:HZ2	1.40	0.67
1:B:35:ARG:NH1	1:B:42:ASP:O	2.27	0.67
1:J:27:ARG:NH2	1:J:49:ASP:O	2.27	0.67
1:K:6:LYS:N	3:K:707:HOH:O	2.28	0.67
1:A:412:ILE:HG23	1:A:620:ILE:HG13	1.77	0.67
1:G:212:HIS:NE2	1:G:447:TYR:OH	2.23	0.66
1:A:58:ILE:HD11	1:B:398:ILE:HG21	1.77	0.66
1:H:133:THR:HG22	1:H:135:THR:H	1.61	0.65
1:C:92:ILE:HD11	1:C:321:ILE:HG12	1.79	0.65
1:B:530:ALA:HB1	1:B:587:ARG:HB3	1.77	0.65
1:E:416:LEU:HB2	1:E:577:TYR:OH	1.95	0.65
1:B:6:LYS:N	3:B:713:HOH:O	2.30	0.65
1:F:33:CYS:SG	3:R:1102:HOH:O	2.54	0.65
1:G:11:ASP:N	1:G:15:ASP:OD2	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:521:GLU:OE2	1:I:545:ARG:NH2	2.30	0.65
1:G:46:THR:HG23	1:G:49:ASP:H	1.62	0.64
1:F:85:ASN:HB2	1:F:327:GLN:HG2	1.78	0.64
1:G:46:THR:HA	1:H:411:ARG:HD2	1.79	0.64
1:A:189:LYS:HE3	1:A:196:PRO:HG3	1.80	0.64
1:J:18:ILE:HD11	1:L:615:ILE:HG21	1.79	0.64
1:C:35:ARG:NH2	3:C:708:HOH:O	2.30	0.63
1:K:436:GLN:O	3:K:701:HOH:O	2.15	0.63
1:G:277:GLN:NE2	3:G:707:HOH:O	2.28	0.63
1:D:291:GLN:O	3:D:701:HOH:O	2.15	0.63
1:E:408:TYR:O	1:E:412:ILE:HG22	1.99	0.63
1:K:584:ASN:ND2	1:L:15:ASP:OD2	2.32	0.63
1:A:351:THR:CB	1:A:362:LEU:HD22	2.24	0.63
1:I:52:ARG:NH1	2:U:996:UNK:O	2.33	0.62
1:B:303:ARG:NH1	1:C:551:ASN:OD1	2.32	0.62
1:I:301:TRP:CH2	1:I:309:ILE:HD11	2.34	0.62
1:B:82:PRO:HG3	1:B:391:ILE:HG22	1.80	0.62
1:J:186:LYS:NZ	3:J:701:HOH:O	2.30	0.62
1:A:175:ARG:NH1	1:A:334:THR:O	2.29	0.62
1:A:527:ARG:HH22	1:A:529:LYS:HE2	1.64	0.62
1:A:398:ILE:HG21	1:C:58:ILE:HD11	1.81	0.62
1:E:94:GLN:OE1	1:E:311:SER:OG	2.13	0.62
1:F:197:LEU:HD21	1:F:618:LEU:HD21	1.79	0.62
1:E:440:LYS:HG3	1:E:441:TRP:CD1	2.35	0.62
1:A:530:ALA:HB1	1:A:587:ARG:HB3	1.82	0.62
1:G:313:SER:HA	1:G:621:SER:HB2	1.82	0.61
1:B:584:ASN:ND2	1:C:15:ASP:OD2	2.29	0.61
1:F:613:LYS:NZ	3:F:708:HOH:O	2.31	0.61
1:I:405:HIS:CE1	1:I:409:ILE:HD11	2.36	0.61
1:D:189:LYS:HD3	1:D:196:PRO:HB3	1.81	0.61
1:B:312:VAL:HG23	1:D:317:GLY:HA3	1.83	0.61
1:D:547:TYR:OH	1:F:303:ARG:NH2	2.34	0.60
1:A:426:ARG:NH2	3:A:709:HOH:O	2.34	0.60
1:D:47:LEU:HD22	1:D:56:LEU:HD11	1.83	0.60
1:A:187:ARG:NH1	1:A:324:ASP:OD2	2.32	0.60
1:B:10:ASN:ND2	1:B:22:ASP:OD2	2.34	0.60
1:J:11:ASP:OD2	1:L:584:ASN:ND2	2.33	0.60
1:E:362:LEU:HG	1:F:492:ASP:HB3	1.83	0.60
1:F:587:ARG:NH2	3:F:711:HOH:O	2.35	0.60
1:C:529:LYS:NZ	3:C:710:HOH:O	2.33	0.60
2:Q:994:UNK:O	2:Q:996:UNK:N	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:33:CYS:SG	3:D:865:HOH:O	2.56	0.59
1:G:354:GLY:O	1:G:357:THR:HG22	2.02	0.59
1:C:193:ASN:H	1:C:318:GLN:HG2	1.66	0.59
1:K:303:ARG:NH2	1:L:547:TYR:OH	2.35	0.59
1:H:234:ALA:HB1	1:H:273:ARG:NH1	2.17	0.59
1:E:584:ASN:ND2	1:F:11:ASP:OD2	2.35	0.59
1:K:126:GLY:N	1:K:139:SER:OG	2.35	0.59
2:Q:991:UNK:N	3:Q:1101:HOH:O	2.32	0.59
2:N:991:UNK:O	3:N:1101:HOH:O	2.17	0.59
1:A:174:VAL:HG23	1:A:289:GLN:HG2	1.85	0.59
1:H:187:ARG:NH1	1:H:324:ASP:OD2	2.35	0.59
1:E:187:ARG:NE	1:E:324:ASP:OD2	2.35	0.58
1:L:110:ALA:O	3:L:701:HOH:O	2.17	0.58
1:L:439:LEU:HD13	1:L:443:VAL:HG21	1.84	0.58
1:H:51:GLU:HA	1:H:54:HIS:O	2.04	0.58
1:E:415:THR:HG22	1:E:618:LEU:HB3	1.85	0.58
1:B:182:LEU:O	3:B:701:HOH:O	2.17	0.58
1:D:102:MET:SD	1:D:321:ILE:HD11	2.44	0.58
1:L:590:GLU:N	1:L:590:GLU:OE1	2.37	0.58
1:G:613:LYS:NZ	3:G:703:HOH:O	2.26	0.57
1:C:182:LEU:HD22	1:C:205:ALA:HB1	1.86	0.57
1:A:101:ASP:HB3	1:A:303:ARG:HG3	1.86	0.57
1:G:75:THR:HG21	1:G:93:PRO:CG	2.32	0.57
1:K:226:GLY:HA3	1:K:294:MET:HE3	1.86	0.57
1:L:533:ILE:HD13	1:L:587:ARG:HH21	1.69	0.57
1:K:51:GLU:OE1	3:K:702:HOH:O	2.17	0.57
1:A:585:ILE:HG22	1:B:11:ASP:HB3	1.85	0.57
1:L:178:GLU:HG3	1:L:465:ARG:HA	1.85	0.57
1:E:440:LYS:HD2	1:E:441:TRP:H	1.70	0.57
1:J:584:ASN:ND2	1:K:15:ASP:OD2	2.36	0.56
1:E:520:THR:OG1	3:E:701:HOH:O	2.18	0.56
1:G:59:ASN:O	3:G:701:HOH:O	2.18	0.56
1:I:183:ARG:HB2	1:I:467:TRP:CZ2	2.41	0.56
1:K:589:ARG:O	1:K:591:PHE:N	2.38	0.56
1:F:27:ARG:HA	2:R:994:UNK:CB	2.35	0.56
1:F:584:ASN:O	1:F:588:ALA:N	2.36	0.56
1:A:189:LYS:HE2	1:A:191:GLU:HG2	1.86	0.56
1:G:313:SER:HB3	1:G:620:ILE:HG23	1.88	0.56
1:G:51:GLU:HA	1:G:54:HIS:O	2.05	0.56
1:C:442:PRO:HB3	1:C:582:HIS:CD2	2.40	0.55
1:E:4:VAL:N	1:F:71:GLU:OE1	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:SER:HB3	1:B:514:TYR:CE1	2.40	0.55
1:E:27:ARG:NH2	1:E:49:ASP:O	2.35	0.55
1:G:33:CYS:SG	3:G:854:HOH:O	2.58	0.55
1:B:51:GLU:HA	1:B:54:HIS:O	2.05	0.55
1:A:334:THR:HG23	1:A:382:ILE:HG23	1.89	0.55
1:E:27:ARG:HH11	2:Q:995:UNK:HA	1.72	0.55
1:F:193:ASN:HA	1:F:318:GLN:NE2	2.22	0.55
1:A:42:ASP:OD2	1:B:411:ARG:NH2	2.39	0.55
1:C:408:TYR:CE1	1:C:412:ILE:HD11	2.42	0.55
1:D:13:LYS:NZ	3:D:715:HOH:O	2.39	0.55
1:E:582:HIS:HE2	1:F:15:ASP:CG	2.09	0.55
1:B:439:LEU:HD13	1:B:443:VAL:HG21	1.89	0.54
1:A:175:ARG:NH2	3:A:706:HOH:O	2.32	0.54
1:B:344:THR:HG22	1:B:370:THR:OG1	2.08	0.54
1:D:63:LYS:HB2	1:F:55:ILE:HG13	1.89	0.54
1:H:364:THR:HG22	1:H:365:GLN:HG3	1.90	0.54
1:I:221:TRP:O	1:I:225:ILE:HG13	2.07	0.54
2:X:1005:UNK:N	3:X:1101:HOH:O	2.33	0.54
1:D:52:ARG:NH2	2:P:996:UNK:O	2.41	0.54
1:G:487:ARG:HB3	1:G:502:PHE:CE1	2.43	0.54
1:E:342:GLN:OE1	3:E:702:HOH:O	2.18	0.54
1:L:13:LYS:HG2	1:L:16:ARG:NH2	2.23	0.54
1:G:524:ASP:HB2	1:G:596:THR:HG22	1.90	0.54
1:J:255:ASP:OD1	1:J:259:THR:N	2.41	0.54
1:A:514:TYR:CE1	1:C:235:SER:HB3	2.43	0.53
1:C:347:THR:OG1	1:C:367:ASN:HB2	2.09	0.53
1:D:27:ARG:NH2	1:D:49:ASP:O	2.41	0.53
1:I:92:ILE:HG23	1:I:395:ILE:HD13	1.89	0.53
1:B:46:THR:HA	1:C:411:ARG:HH11	1.72	0.53
1:J:326:GLU:OE1	3:J:701:HOH:O	2.18	0.53
1:J:52:ARG:NH2	2:V:996:UNK:O	2.41	0.53
1:E:303:ARG:NH1	1:F:551:ASN:OD1	2.37	0.53
1:K:51:GLU:HA	1:K:54:HIS:O	2.09	0.53
1:A:24:LEU:HB2	1:A:54:HIS:CE1	2.44	0.53
1:B:312:VAL:HG11	1:B:409:ILE:HG12	1.91	0.53
1:I:573:TYR:O	1:I:576:THR:OG1	2.24	0.53
1:K:89:GLN:HG3	1:K:322:THR:HG22	1.91	0.53
1:A:432:ASP:OD1	1:A:433:GLN:N	2.42	0.53
1:H:392:GLU:OE1	3:H:701:HOH:O	2.19	0.52
1:J:357:THR:HG22	1:J:359:THR:H	1.74	0.52
1:G:221:TRP:O	1:G:225:ILE:HG13	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:58:ILE:HD11	1:H:398:ILE:HG21	1.91	0.52
1:H:221:TRP:O	1:H:225:ILE:HG13	2.09	0.52
1:B:364:THR:HG22	1:B:365:GLN:HG3	1.91	0.52
1:E:490:ILE:HD13	1:E:503:LYS:HE2	1.92	0.52
1:A:46:THR:HG22	1:A:48:VAL:N	2.22	0.52
1:C:24:LEU:HB2	1:C:54:HIS:CE1	2.44	0.52
1:E:238:VAL:HG11	1:E:274:LYS:HE3	1.92	0.52
1:E:105:HIS:O	1:E:391:ILE:HA	2.09	0.52
1:L:48:VAL:O	1:L:52:ARG:HG3	2.10	0.52
1:F:48:VAL:O	1:F:52:ARG:HG3	2.09	0.52
1:B:620:ILE:HG22	1:B:621:SER:HB3	1.92	0.52
1:C:28:ILE:HA	1:C:31:ILE:HG22	1.90	0.52
1:D:51:GLU:HA	1:D:54:HIS:O	2.10	0.52
1:G:82:PRO:HG3	1:G:391:ILE:HG22	1.92	0.52
1:E:436:GLN:HB2	1:E:591:PHE:HB3	1.92	0.52
1:F:585:ILE:HD12	1:F:585:ILE:H	1.75	0.51
1:H:235:SER:HB3	1:I:514:TYR:CE2	2.45	0.51
1:J:275:LEU:HB2	1:K:277:GLN:HB2	1.92	0.51
1:G:92:ILE:HG23	1:G:395:ILE:HD13	1.92	0.51
1:K:584:ASN:HD22	1:L:15:ASP:CG	2.14	0.51
1:A:527:ARG:NH1	1:A:529:LYS:HE2	2.18	0.51
1:D:235:SER:HB3	1:E:514:TYR:CD2	2.44	0.51
1:K:31:ILE:HG13	3:W:1101:HOH:O	2.10	0.51
1:G:291:GLN:NE2	1:G:389:GLN:OE1	2.39	0.51
1:I:585:ILE:HA	1:I:588:ALA:HB3	1.91	0.51
1:C:487:ARG:HB3	1:C:502:PHE:CE1	2.46	0.51
1:H:182:LEU:HD22	1:H:205:ALA:HB1	1.92	0.51
1:E:58:ILE:HD11	1:F:398:ILE:HG21	1.92	0.51
1:L:545:ARG:HD2	1:L:563:LYS:HA	1.92	0.51
1:J:182:LEU:HD22	1:J:205:ALA:HB1	1.93	0.51
1:B:350:THR:HB	3:B:703:HOH:O	2.11	0.51
1:C:487:ARG:NE	1:C:504:GLN:HG2	2.26	0.50
1:E:172:ASN:ND2	1:E:380:SER:HB3	2.25	0.50
1:G:432:ASP:OD1	1:G:433:GLN:N	2.44	0.50
1:A:527:ARG:NH1	1:A:529:LYS:CG	2.74	0.50
1:D:102:MET:HG2	1:D:395:ILE:HG12	1.93	0.50
1:E:13:LYS:HE3	2:Q:1009:UNK:O	2.12	0.50
1:G:409:ILE:HG23	1:G:620:ILE:HG21	1.92	0.50
1:J:44:THR:O	1:K:411:ARG:NH2	2.29	0.50
1:A:24:LEU:HD21	1:B:404:ILE:HD11	1.92	0.50
1:B:487:ARG:HD3	1:B:502:PHE:CZ	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:ILE:HG12	1:C:45:PRO:HD2	1.92	0.50
1:F:183:ARG:HB2	1:F:467:TRP:CZ2	2.46	0.50
1:I:51:GLU:HA	1:I:54:HIS:O	2.12	0.50
1:A:132:LEU:HD13	1:A:137:VAL:HG22	1.93	0.50
1:D:57:LEU:HD13	1:F:572:LEU:HD12	1.93	0.50
1:G:486:ALA:HB3	1:G:505:SER:HB3	1.93	0.50
1:K:31:ILE:O	1:K:35:ARG:HG3	2.11	0.50
1:E:79:THR:HG21	1:E:88:ILE:HA	1.93	0.50
1:C:183:ARG:HB2	1:C:467:TRP:CZ2	2.47	0.50
1:K:157:VAL:HG12	1:K:158:ASN:O	2.11	0.50
1:K:6:LYS:HE3	1:K:8:ILE:HD11	1.94	0.50
1:A:487:ARG:HB3	1:A:502:PHE:CE1	2.47	0.50
1:H:16:ARG:NH2	3:H:712:HOH:O	2.32	0.50
1:L:92:ILE:HG23	1:L:395:ILE:HD13	1.94	0.50
1:G:27:ARG:O	1:G:31:ILE:HG22	2.12	0.50
1:J:587:ARG:HH21	1:K:6:LYS:HE3	1.77	0.49
1:J:540:ARG:NH2	3:J:715:HOH:O	2.41	0.49
2:R:991:UNK:HA	3:R:1102:HOH:O	2.12	0.49
2:X:1006:UNK:N	3:X:1101:HOH:O	2.35	0.49
1:A:351:THR:HG1	1:A:362:LEU:CD2	2.18	0.49
1:A:347:THR:OG1	1:A:367:ASN:HB2	2.11	0.49
1:I:154:GLN:HA	1:I:342:GLN:O	2.11	0.49
1:G:235:SER:HB3	1:H:514:TYR:CE1	2.48	0.49
1:B:105:HIS:O	1:B:391:ILE:HA	2.13	0.49
1:B:478:VAL:HB	1:B:514:TYR:HB2	1.94	0.49
1:F:30:SER:OG	2:R:994:UNK:O	2.29	0.49
1:F:439:LEU:HD13	1:F:443:VAL:HG21	1.95	0.49
1:F:46:THR:OG1	1:F:49:ASP:N	2.41	0.49
1:D:140:ALA:HB2	1:D:151:LEU:HD12	1.95	0.49
1:D:530:ALA:O	1:D:533:ILE:HG13	2.13	0.49
1:I:553:GLY:HA2	1:I:574:PRO:O	2.13	0.49
1:J:514:TYR:CE2	1:L:235:SER:HB3	2.48	0.48
1:K:189:LYS:HG2	1:K:191:GLU:HG3	1.95	0.48
1:A:471:THR:HB	1:A:520:THR:O	2.13	0.48
1:C:418:ARG:NH2	1:C:577:TYR:O	2.45	0.48
1:J:439:LEU:HD13	1:J:443:VAL:HG21	1.94	0.48
1:C:530:ALA:O	1:C:533:ILE:HG12	2.14	0.48
1:F:209:ASN:OD1	1:F:221:TRP:NE1	2.40	0.48
1:G:398:ILE:HG21	1:I:58:ILE:HD11	1.94	0.48
1:E:45:PRO:HG2	1:F:407:ILE:HD13	1.96	0.48
1:C:318:GLN:HG2	1:C:318:GLN:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:105:HIS:O	1:F:391:ILE:HA	2.14	0.48
1:K:188:VAL:HG11	1:K:298:LEU:HD22	1.94	0.48
1:I:152:TYR:HD1	1:I:345:VAL:HG22	1.79	0.48
1:I:421:ARG:HD3	1:I:441:TRP:CZ3	2.49	0.48
1:A:221:TRP:O	1:A:225:ILE:HG13	2.14	0.48
1:A:486:ALA:HB3	1:A:505:SER:HB3	1.95	0.48
1:D:432:ASP:OD1	1:D:433:GLN:N	2.46	0.48
1:I:435:LEU:HD13	1:I:592:TYR:HE1	1.79	0.48
1:D:405:HIS:O	1:D:409:ILE:HG12	2.14	0.48
1:L:533:ILE:HD13	1:L:587:ARG:NH2	2.28	0.48
1:A:527:ARG:NH2	1:A:529:LYS:HE2	2.28	0.48
1:A:44:THR:HG21	1:B:410:LYS:HD2	1.96	0.48
1:E:228:GLU:OE2	1:E:284:THR:HG23	2.13	0.48
1:G:620:ILE:HA	1:G:621:SER:HA	1.64	0.48
1:I:193:ASN:ND2	1:I:318:GLN:OE1	2.46	0.48
1:D:270:ILE:HG12	1:F:476:GLU:HG2	1.95	0.48
1:G:346:GLU:OE1	1:G:366:TYR:OH	2.26	0.48
1:C:545:ARG:NH1	1:C:546:ASP:OD2	2.45	0.47
1:F:442:PRO:HG3	1:F:585:ILE:HD11	1.96	0.47
1:J:82:PRO:HG3	1:J:391:ILE:HG22	1.96	0.47
1:L:105:HIS:O	1:L:391:ILE:HA	2.14	0.47
1:C:414:PHE:HB3	1:C:619:LEU:HD23	1.95	0.47
1:L:141:THR:HG23	1:L:152:TYR:HE2	1.80	0.47
1:L:183:ARG:HB2	1:L:467:TRP:CZ2	2.49	0.47
1:A:407:ILE:HD13	1:C:50:ILE:HD11	1.97	0.47
1:G:27:ARG:HA	2:S:994:UNK:CB	2.44	0.47
1:A:527:ARG:NH1	1:A:529:LYS:HG3	2.29	0.47
1:B:477:PRO:HB3	1:B:513:GLN:HE21	1.80	0.47
1:C:412:ILE:HD13	1:C:412:ILE:HG21	1.72	0.47
1:E:192:VAL:HG13	1:E:314:ILE:HG23	1.95	0.47
1:A:175:ARG:NH1	1:A:335:ALA:HB2	2.25	0.47
1:B:182:LEU:HD22	1:B:205:ALA:HB1	1.95	0.47
1:C:456:ILE:HA	1:C:463:GLN:HG3	1.97	0.47
1:F:569:ASN:ND2	1:F:571:CYS:O	2.43	0.47
1:K:172:ASN:ND2	1:K:380:SER:HB3	2.30	0.47
1:A:362:LEU:HD23	1:A:362:LEU:O	2.14	0.47
1:G:487:ARG:HB2	1:I:366:TYR:CD2	2.49	0.47
1:A:527:ARG:HH12	1:A:529:LYS:CG	2.28	0.47
1:C:51:GLU:HA	1:C:54:HIS:O	2.15	0.47
1:D:152:TYR:HD1	1:D:345:VAL:HG22	1.80	0.47
1:H:360:GLY:O	1:I:496:PRO:HD2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:44:THR:HG21	1:L:410:LYS:HD3	1.95	0.47
1:K:415:THR:OG1	1:K:618:LEU:HB3	2.14	0.47
1:L:24:LEU:O	1:L:28:ILE:HG12	2.15	0.47
1:L:27:ARG:NH2	1:L:49:ASP:O	2.45	0.47
1:K:57:LEU:HD12	1:L:68:MET:HE2	1.97	0.47
1:D:60:SER:OG	1:E:412:ILE:HD11	2.14	0.47
1:G:572:LEU:HD12	1:H:57:LEU:HD13	1.96	0.47
1:H:383:ASP:OD1	1:H:385:THR:OG1	2.24	0.47
1:H:24:LEU:HD21	1:I:404:ILE:HD11	1.97	0.47
1:J:414:PHE:HB3	1:J:619:LEU:HD23	1.97	0.47
1:F:531:HIS:CD2	1:F:587:ARG:HA	2.50	0.47
1:I:351:THR:OG1	1:I:362:LEU:HD22	2.15	0.47
1:J:235:SER:HB3	1:K:514:TYR:CE2	2.50	0.47
2:W:993:UNK:O	2:W:995:UNK:N	2.48	0.47
1:A:412:ILE:CG2	1:A:620:ILE:HG13	2.44	0.47
1:A:62:TYR:CE1	1:B:416:LEU:HD13	2.50	0.46
1:B:94:GLN:HE22	1:D:315:PRO:HA	1.80	0.46
1:C:82:PRO:HG3	1:C:391:ILE:HG22	1.97	0.46
1:I:50:ILE:HG21	1:I:56:LEU:HD21	1.97	0.46
1:F:285:PRO:HB3	1:F:335:ALA:HB3	1.98	0.46
1:G:373:THR:O	1:G:375:THR:HG23	2.15	0.46
1:I:13:LYS:O	1:I:17:MET:HG3	2.16	0.46
1:J:152:TYR:HD1	1:J:345:VAL:HG22	1.79	0.46
1:L:102:MET:O	1:L:303:ARG:NH2	2.48	0.46
1:B:347:THR:OG1	1:B:367:ASN:HB2	2.16	0.46
1:K:187:ARG:NH2	1:K:324:ASP:OD2	2.48	0.46
1:C:352:GLY:HA3	1:C:361:VAL:HG23	1.96	0.46
1:F:111:THR:HG21	1:F:386:GLN:HB2	1.96	0.46
1:J:105:HIS:O	1:J:391:ILE:HA	2.16	0.46
1:J:189:LYS:HD2	1:J:191:GLU:HG3	1.95	0.46
1:K:189:LYS:NZ	1:K:322:THR:OG1	2.46	0.46
1:L:442:PRO:HD3	1:L:585:ILE:HG12	1.96	0.46
1:D:238:VAL:HG11	1:D:274:LYS:HE2	1.98	0.46
1:D:529:LYS:HG2	1:D:592:TYR:HB2	1.98	0.46
1:D:60:SER:HB2	1:E:415:THR:OG1	2.16	0.46
1:J:587:ARG:HH21	1:K:6:LYS:CE	2.29	0.46
1:C:537:ALA:HB3	1:C:539:TYR:CZ	2.51	0.46
1:G:149:TYR:HD2	1:G:348:LEU:HD12	1.81	0.46
1:C:221:TRP:O	1:C:225:ILE:HG12	2.14	0.46
1:C:411:ARG:HA	1:C:411:ARG:HD3	1.71	0.46
1:E:411:ARG:HA	1:E:411:ARG:HD3	1.75	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:398:ILE:HG21	1:F:58:ILE:HD11	1.97	0.46
1:H:37:LYS:NZ	3:H:720:HOH:O	2.39	0.46
1:L:203:LEU:HD13	1:L:609:ILE:HG12	1.96	0.46
1:C:334:THR:HG21	1:C:381:SER:HA	1.98	0.46
1:E:157:VAL:HG12	1:E:158:ASN:O	2.15	0.46
1:I:544:TYR:HB2	1:I:566:LEU:HD23	1.98	0.46
1:D:604:ASN:ND2	3:D:707:HOH:O	2.33	0.46
1:J:197:LEU:HD11	1:J:618:LEU:HD11	1.97	0.46
1:K:180:PRO:HD2	1:K:225:ILE:O	2.15	0.46
1:K:295:PHE:O	1:K:297:PRO:HD3	2.16	0.46
1:K:95:PHE:HB3	1:K:397:ASN:OD1	2.16	0.46
1:G:135:THR:HB	1:G:163:THR:HG21	1.97	0.46
1:G:416:LEU:HD21	1:G:615:ILE:HG23	1.97	0.46
1:H:442:PRO:HA	1:H:583:VAL:O	2.16	0.46
1:J:51:GLU:HA	1:J:54:HIS:O	2.16	0.46
1:B:531:HIS:ND1	1:B:531:HIS:O	2.48	0.45
1:F:154:GLN:HA	1:F:342:GLN:O	2.15	0.45
1:J:398:ILE:HG21	1:L:58:ILE:HD11	1.97	0.45
1:K:183:ARG:HB2	1:K:467:TRP:CZ2	2.51	0.45
1:I:530:ALA:O	1:I:533:ILE:HG13	2.15	0.45
1:B:221:TRP:O	1:B:225:ILE:HG12	2.16	0.45
1:B:438:GLN:HG2	1:B:439:LEU:HD23	1.99	0.45
1:K:124:PHE:CE1	1:K:130:GLN:HB3	2.52	0.45
1:K:76:ARG:HH12	1:K:390:ASN:ND2	2.13	0.45
1:G:31:ILE:HG23	1:G:45:PRO:HG3	1.97	0.45
1:H:503:LYS:HG3	1:I:488:VAL:HG13	1.97	0.45
1:B:31:ILE:O	1:B:35:ARG:HG3	2.15	0.45
1:H:529:LYS:NZ	3:H:726:HOH:O	2.43	0.45
1:H:587:ARG:NH2	1:I:6:LYS:O	2.38	0.45
1:J:255:ASP:OD1	1:J:258:GLY:N	2.49	0.45
1:J:540:ARG:NH1	3:J:724:HOH:O	2.49	0.45
1:A:215:ASP:HA	1:A:218:LEU:HB2	1.99	0.45
1:D:321:ILE:HD12	1:D:393:LEU:HD21	1.98	0.45
1:F:491:ASP:HB3	1:F:494:VAL:HG22	1.99	0.45
1:H:347:THR:OG1	1:H:367:ASN:HB2	2.17	0.45
1:B:177:CYS:O	1:B:180:PRO:HD3	2.16	0.45
1:B:432:ASP:OD1	1:B:433:GLN:N	2.46	0.45
1:F:585:ILE:HA	1:F:588:ALA:HB3	1.99	0.45
1:I:190:PHE:CE2	1:I:197:LEU:HD23	2.52	0.45
1:K:221:TRP:O	1:K:225:ILE:HG12	2.17	0.45
1:C:156:TYR:HB3	1:C:339:LEU:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:203:LEU:HB3	1:C:611:ILE:HD11	1.98	0.45
1:J:189:LYS:HD3	1:J:196:PRO:HB3	1.99	0.45
1:D:112:SER:HB3	1:D:288:THR:HG22	1.99	0.45
1:F:121:LEU:HD13	1:F:137:VAL:HG23	1.99	0.45
1:G:95:PHE:HB3	1:G:397:ASN:OD1	2.17	0.45
1:K:46:THR:HG23	1:K:49:ASP:H	1.82	0.45
1:L:121:LEU:HD13	1:L:137:VAL:HG23	1.98	0.45
1:L:135:THR:HB	1:L:163:THR:HG21	1.99	0.45
1:H:477:PRO:HB3	1:H:513:GLN:HE21	1.81	0.44
1:D:96:GLY:HA2	1:D:399:PHE:CE1	2.52	0.44
1:E:63:LYS:HG3	1:E:64:PRO:HD2	1.98	0.44
1:G:182:LEU:HD21	1:G:221:TRP:HZ2	1.81	0.44
1:L:75:THR:HG21	1:L:93:PRO:CG	2.47	0.44
1:D:189:LYS:HD2	1:D:191:GLU:HG2	1.99	0.44
1:D:480:ASP:OD1	1:E:274:LYS:NZ	2.42	0.44
1:J:187:ARG:NH1	1:J:324:ASP:OD2	2.45	0.44
1:J:442:PRO:HB3	1:J:582:HIS:CD2	2.52	0.44
1:J:448:LEU:HD11	1:J:608:LEU:HD11	1.99	0.44
1:E:295:PHE:O	1:E:297:PRO:HD3	2.16	0.44
1:A:487:ARG:HB2	1:C:366:TYR:CD2	2.52	0.44
1:D:255:ASP:OD1	1:D:258:GLY:N	2.51	0.44
1:G:134:SER:HB2	1:G:165:THR:HG23	1.99	0.44
1:G:440:LYS:O	1:G:585:ILE:HD11	2.17	0.44
1:I:29:LYS:HG3	1:I:30:SER:N	2.32	0.44
1:K:101:ASP:HB2	1:K:303:ARG:NH2	2.32	0.44
1:D:189:LYS:HD2	1:D:191:GLU:CG	2.47	0.44
1:J:27:ARG:HD2	2:V:994:UNK:O	2.18	0.44
1:H:94:GLN:OE1	1:J:315:PRO:HA	2.18	0.44
1:L:412:ILE:CG2	1:L:620:ILE:HG13	2.47	0.44
1:H:95:PHE:HB3	1:H:397:ASN:OD1	2.18	0.44
1:A:279:VAL:HG13	1:C:275:LEU:HD21	2.00	0.44
1:B:47:LEU:HD11	1:C:412:ILE:HG13	1.99	0.44
1:E:613:LYS:NZ	3:E:732:HOH:O	2.51	0.44
1:F:406:ASP:OD2	1:F:410:LYS:NZ	2.50	0.44
1:G:124:PHE:CZ	1:G:130:GLN:HB3	2.53	0.44
1:I:124:PHE:CE1	1:I:130:GLN:HB3	2.53	0.44
1:D:304:ASP:OD1	1:D:306:ARG:HG2	2.17	0.44
1:E:24:LEU:HD21	1:F:404:ILE:HD11	2.00	0.44
1:L:51:GLU:HA	1:L:54:HIS:O	2.18	0.44
1:B:192:VAL:HG21	1:B:314:ILE:HD13	2.01	0.43
1:I:545:ARG:HD2	1:I:546:ASP:OD1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:312:VAL:HG23	1:D:317:GLY:CA	2.47	0.43
1:E:174:VAL:HG23	1:E:289:GLN:HG2	1.99	0.43
1:E:57:LEU:HD12	1:F:68:MET:HE2	1.99	0.43
1:F:527:ARG:HD3	1:F:594:GLU:OE2	2.17	0.43
1:H:315:PRO:HB3	1:J:318:GLN:OE1	2.17	0.43
1:I:436:GLN:HB2	1:I:591:PHE:HB3	2.00	0.43
1:I:613:LYS:HD2	1:I:613:LYS:HA	1.73	0.43
1:L:326:GLU:OE1	3:L:703:HOH:O	2.21	0.43
1:A:589:ARG:HG2	1:A:589:ARG:O	2.18	0.43
1:H:289:GLN:OE1	3:H:702:HOH:O	2.20	0.43
1:I:529:LYS:HE2	1:I:532:GLY:HA2	2.00	0.43
1:L:75:THR:HG21	1:L:93:PRO:HG2	2.01	0.43
1:B:235:SER:HB3	1:C:514:TYR:CE2	2.54	0.43
1:E:183:ARG:HB2	1:E:467:TRP:CZ2	2.53	0.43
1:F:422:GLU:HG3	1:F:611:ILE:HG12	2.00	0.43
1:L:285:PRO:HB3	1:L:335:ALA:HB3	1.99	0.43
1:L:485:TYR:O	3:L:702:HOH:O	2.21	0.43
2:X:1002:UNK:C	3:X:1101:HOH:O	2.66	0.43
1:B:459:GLY:N	3:B:716:HOH:O	2.31	0.43
1:C:154:GLN:HA	1:C:342:GLN:O	2.19	0.43
1:D:531:HIS:HB2	1:D:587:ARG:HA	2.00	0.43
1:B:466:ASP:OD2	3:B:702:HOH:O	2.21	0.43
1:I:477:PRO:HB3	1:I:513:GLN:NE2	2.34	0.43
1:J:404:ILE:HD11	1:L:24:LEU:HD21	2.00	0.43
1:L:101:ASP:HB2	1:L:303:ARG:NH1	2.33	0.43
1:L:415:THR:HG23	1:L:618:LEU:HB2	2.00	0.43
1:A:51:GLU:HA	1:A:54:HIS:O	2.19	0.43
1:B:30:SER:O	1:B:34:LEU:HD13	2.18	0.43
1:G:309:ILE:HG21	1:G:314:ILE:HD12	2.00	0.43
1:H:212:HIS:NE2	1:H:447:TYR:OH	2.26	0.43
1:L:412:ILE:HG23	1:L:620:ILE:HG13	2.00	0.43
1:E:13:LYS:HG2	1:E:17:MET:HE2	2.01	0.43
1:E:275:LEU:HB2	1:F:277:GLN:HB2	2.01	0.43
1:G:154:GLN:HA	1:G:342:GLN:O	2.18	0.43
1:K:96:GLY:HA2	1:K:399:PHE:CE2	2.54	0.43
1:L:347:THR:OG1	1:L:367:ASN:HB2	2.18	0.43
2:R:993:UNK:O	2:R:995:UNK:N	2.52	0.43
1:C:571:CYS:HB3	1:C:581:GLY:O	2.19	0.43
1:D:154:GLN:HA	1:D:342:GLN:O	2.19	0.43
1:E:499:SER:OG	1:E:501:THR:HG22	2.19	0.43
1:E:585:ILE:HD12	1:E:589:ARG:HH21	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:476:GLU:HG2	1:I:270:ILE:HG12	2.00	0.43
1:J:529:LYS:NZ	1:J:594:GLU:OE2	2.43	0.43
1:K:220:GLY:O	1:K:224:LEU:HG	2.19	0.43
1:C:418:ARG:NH1	1:C:444:GLU:OE1	2.52	0.43
1:B:57:LEU:HD12	1:C:68:MET:HG2	2.01	0.43
1:D:95:PHE:HB3	1:D:397:ASN:OD1	2.18	0.43
1:H:46:THR:HG23	1:H:49:ASP:H	1.83	0.43
1:K:108:LEU:HD12	1:K:292:LEU:HD23	2.01	0.43
1:K:24:LEU:HD21	1:L:404:ILE:HD11	2.00	0.43
3:L:834:HOH:O	2:X:991:UNK:HA	2.19	0.43
1:A:530:ALA:CB	1:A:587:ARG:HB3	2.49	0.42
1:E:585:ILE:HG13	1:E:586:SER:N	2.33	0.42
1:J:223:ARG:NH1	3:K:709:HOH:O	2.52	0.42
1:J:272:ALA:HB1	1:K:278:VAL:HG13	2.01	0.42
1:C:512:ASN:OD1	1:C:513:GLN:N	2.47	0.42
1:D:442:PRO:HB3	1:D:582:HIS:CD2	2.54	0.42
1:C:13:LYS:O	1:C:17:MET:HG3	2.19	0.42
1:D:487:ARG:HB3	1:D:502:PHE:CE1	2.55	0.42
1:G:23:LEU:O	1:G:27:ARG:HG3	2.20	0.42
1:K:219:THR:O	1:K:223:ARG:HG3	2.19	0.42
1:K:616:ASN:OD1	1:K:617:PHE:N	2.46	0.42
1:J:261:VAL:HG21	1:L:125:ILE:HD12	2.01	0.42
1:J:407:ILE:CD1	1:L:45:PRO:HG2	2.49	0.42
1:L:487:ARG:HD2	1:L:504:GLN:HA	2.00	0.42
1:L:210:LYS:NZ	1:L:562:ASP:OD2	2.52	0.42
1:G:450:LEU:HB3	1:G:522:THR:OG1	2.19	0.42
1:J:180:PRO:HD2	1:J:225:ILE:O	2.20	0.42
1:A:404:ILE:HD11	1:C:24:LEU:HD21	2.00	0.42
1:A:416:LEU:HD11	1:A:579:PRO:HG3	2.01	0.42
1:A:474:THR:CG2	1:A:518:VAL:HB	2.49	0.42
1:C:554:SER:OG	1:C:555:PHE:N	2.53	0.42
1:G:526:VAL:HB	1:G:544:TYR:CE2	2.54	0.42
1:I:405:HIS:ND1	1:I:409:ILE:HD11	2.35	0.42
1:J:587:ARG:NH2	1:K:6:LYS:O	2.51	0.42
1:H:289:GLN:HG3	3:H:724:HOH:O	2.20	0.42
1:H:201:THR:OG1	1:H:422:GLU:OE1	2.31	0.42
1:J:55:ILE:HD11	1:K:63:LYS:HB2	2.00	0.42
1:L:487:ARG:NE	1:L:504:GLN:HG2	2.35	0.42
1:A:193:ASN:ND2	1:A:318:GLN:OE1	2.53	0.42
1:B:238:VAL:HG11	1:B:274:LYS:HD3	2.02	0.42
1:G:94:GLN:OE1	1:G:311:SER:OG	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:48:VAL:O	1:I:52:ARG:HG3	2.19	0.42
1:A:105:HIS:O	1:A:391:ILE:HA	2.20	0.42
1:I:537:ALA:HB3	1:I:539:TYR:CZ	2.54	0.42
1:K:55:ILE:HA	1:K:55:ILE:HD12	1.97	0.42
1:A:307:LEU:HD11	1:A:577:TYR:CD1	2.55	0.42
1:D:585:ILE:HD12	1:D:589:ARG:HH21	1.84	0.42
1:F:85:ASN:CB	1:F:327:GLN:HG2	2.48	0.42
1:H:527:ARG:NH1	1:H:534:GLU:OE2	2.51	0.42
1:A:279:VAL:HG23	1:C:273:ARG:HG3	2.01	0.42
1:D:277:GLN:HB2	1:F:275:LEU:HB2	2.02	0.42
1:H:557:LEU:HD12	1:H:557:LEU:HA	1.90	0.42
1:C:476:GLU:HB3	1:C:516:VAL:HB	2.01	0.41
1:C:585:ILE:HG13	1:C:586:SER:N	2.33	0.41
1:D:235:SER:HB3	1:E:514:TYR:CE2	2.55	0.41
1:I:574:PRO:HA	1:I:575:GLY:HA2	1.70	0.41
1:D:273:ARG:NE	1:E:284:THR:HG22	2.19	0.41
1:G:140:ALA:HB2	1:G:151:LEU:HD12	2.03	0.41
1:H:183:ARG:HB2	1:H:467:TRP:CZ2	2.55	0.41
1:I:24:LEU:HB2	1:I:54:HIS:CE1	2.55	0.41
1:C:31:ILE:CG2	1:C:45:PRO:HG3	2.51	0.41
1:D:82:PRO:HG3	1:D:391:ILE:HG22	2.02	0.41
1:D:44:THR:C	1:E:411:ARG:HH21	2.18	0.41
1:G:407:ILE:HG12	1:I:45:PRO:HD2	2.02	0.41
1:H:6:LYS:HA	1:H:6:LYS:HD3	1.90	0.41
1:G:436:GLN:HB2	1:G:591:PHE:HB3	2.03	0.41
1:I:347:THR:OG1	1:I:367:ASN:HB2	2.21	0.41
1:A:527:ARG:CZ	1:A:529:LYS:CE	2.93	0.41
1:D:545:ARG:HD2	1:D:546:ASP:OD1	2.21	0.41
1:F:31:ILE:HD13	1:F:49:ASP:HB3	2.01	0.41
1:I:200:TYR:HB2	1:I:204:ALA:HB3	2.02	0.41
1:G:411:ARG:NH2	1:I:44:THR:O	2.49	0.41
1:K:174:VAL:HG23	1:K:289:GLN:HG2	2.02	0.41
1:B:133:THR:HG22	1:B:134:SER:H	1.86	0.41
1:E:216:PHE:HB2	1:F:558:VAL:HG22	2.02	0.41
1:H:585:ILE:O	1:H:589:ARG:HG3	2.21	0.41
1:J:124:PHE:CE1	1:J:130:GLN:HB3	2.56	0.41
1:J:599:PHE:CE2	1:J:604:ASN:HB3	2.55	0.41
1:L:154:GLN:HA	1:L:342:GLN:O	2.20	0.41
1:L:24:LEU:HD13	1:L:54:HIS:CG	2.56	0.41
1:A:309:ILE:HG21	1:A:314:ILE:HD12	2.02	0.41
1:A:46:THR:HA	1:B:411:ARG:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:THR:HG22	1:B:134:SER:N	2.36	0.41
1:C:417:ILE:HG21	1:C:618:LEU:HD13	2.02	0.41
1:D:244:THR:HG21	1:D:251:VAL:HG21	2.03	0.41
1:D:449:GLY:HA3	1:D:470:LEU:HD13	2.02	0.41
1:E:51:GLU:HA	1:E:54:HIS:O	2.21	0.41
1:I:239:ASN:O	1:I:271:THR:HA	2.20	0.41
1:J:27:ARG:HH11	2:V:995:UNK:HA	1.84	0.41
1:K:361:VAL:O	1:K:362:LEU:HB3	2.20	0.41
1:C:105:HIS:O	1:C:391:ILE:HA	2.21	0.41
1:C:421:ARG:HD3	1:C:441:TRP:HZ3	1.86	0.41
1:G:466:ASP:OD2	3:G:702:HOH:O	2.21	0.41
1:H:416:LEU:HB2	1:H:577:TYR:CE1	2.56	0.41
1:L:434:VAL:HG11	1:L:608:LEU:HD23	2.03	0.41
1:E:255:ASP:OD2	1:E:259:THR:HB	2.20	0.41
1:K:347:THR:OG1	1:K:367:ASN:HB2	2.21	0.41
1:L:438:GLN:HG3	1:L:438:GLN:O	2.21	0.41
1:B:239:ASN:O	1:B:271:THR:HA	2.21	0.41
1:C:186:LYS:HD2	1:C:326:GLU:HA	2.02	0.41
1:E:571:CYS:HB3	1:E:581:GLY:O	2.21	0.41
1:L:531:HIS:NE2	1:L:586:SER:O	2.53	0.41
1:A:172:ASN:ND2	1:A:380:SER:HB3	2.35	0.41
1:B:174:VAL:HG23	1:B:289:GLN:HB2	2.01	0.41
1:B:615:ILE:HG21	1:C:18:ILE:HD11	2.03	0.41
1:C:472:SER:HB3	1:C:520:THR:HB	2.02	0.41
1:D:238:VAL:HG22	1:D:273:ARG:HA	2.02	0.41
1:E:31:ILE:O	1:E:35:ARG:HG3	2.21	0.41
1:E:450:LEU:HD13	1:E:608:LEU:HD23	2.01	0.41
1:I:435:LEU:HD13	1:I:592:TYR:CE1	2.56	0.41
1:K:512:ASN:OD1	1:K:513:GLN:N	2.48	0.41
1:L:221:TRP:O	1:L:225:ILE:HG12	2.21	0.41
1:C:442:PRO:HD3	1:C:585:ILE:HG22	2.03	0.40
1:D:47:LEU:HA	1:D:47:LEU:HD23	1.79	0.40
1:E:426:ARG:HD3	1:E:427:GLU:H	1.86	0.40
1:I:23:LEU:O	1:I:27:ARG:HG3	2.20	0.40
1:I:477:PRO:HB3	1:I:513:GLN:HE21	1.86	0.40
1:J:24:LEU:HB2	1:J:54:HIS:CE1	2.56	0.40
2:X:1008:UNK:HA	3:X:1102:HOH:O	2.21	0.40
1:A:189:LYS:CE	1:A:196:PRO:HG3	2.49	0.40
1:F:463:GLN:HB3	1:F:463:GLN:HE21	1.60	0.40
1:H:275:LEU:HD12	1:I:230:PRO:HB3	2.03	0.40
1:H:124:PHE:O	1:I:255:ASP:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:515:ILE:HA	1:I:515:ILE:HD13	1.97	0.40
1:J:304:ASP:OD1	1:J:306:ARG:HG2	2.20	0.40
1:B:183:ARG:HB2	1:B:467:TRP:CZ2	2.56	0.40
1:B:46:THR:HA	1:C:411:ARG:NH1	2.36	0.40
1:B:487:ARG:HG2	1:B:503:LYS:O	2.22	0.40
1:B:95:PHE:HB3	1:B:397:ASN:OD1	2.22	0.40
1:C:423:GLN:OE1	1:C:437:SER:N	2.54	0.40
1:F:416:LEU:HD12	1:F:617:PHE:CE1	2.56	0.40
1:H:235:SER:O	1:H:273:ARG:HD2	2.21	0.40
1:J:476:GLU:HG2	1:K:270:ILE:HG12	2.04	0.40
1:L:238:VAL:HG11	1:L:274:LYS:HD2	2.02	0.40
1:L:154:GLN:HG2	1:L:343:THR:HA	2.03	0.40
1:B:613:LYS:HD2	1:B:613:LYS:HA	1.79	0.40
1:E:221:TRP:O	1:E:225:ILE:HG12	2.21	0.40
1:E:445:PHE:CE1	1:E:613:LYS:HG3	2.57	0.40
1:H:601:ASP:OD1	1:H:603:SER:N	2.55	0.40
1:F:530:ALA:HB1	1:F:587:ARG:O	2.22	0.40
1:H:24:LEU:O	1:H:28:ILE:HG13	2.22	0.40
1:J:206:ILE:O	1:J:210:LYS:HG3	2.21	0.40
1:K:149:TYR:CZ	1:K:358:ALA:HB2	2.56	0.40
1:K:418:ARG:HE	1:K:444:GLU:CD	2.25	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	607/645 (94%)	593 (98%)	14 (2%)	0	100	100
1	B	614/645 (95%)	597 (97%)	17 (3%)	0	100	100
1	C	614/645 (95%)	598 (97%)	16 (3%)	0	100	100
1	D	607/645 (94%)	591 (97%)	16 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	614/645 (95%)	597 (97%)	17 (3%)	0	100	100
1	F	608/645 (94%)	583 (96%)	25 (4%)	0	100	100
1	G	609/645 (94%)	592 (97%)	17 (3%)	0	100	100
1	H	613/645 (95%)	593 (97%)	20 (3%)	0	100	100
1	I	614/645 (95%)	596 (97%)	18 (3%)	0	100	100
1	J	608/645 (94%)	592 (97%)	16 (3%)	0	100	100
1	K	612/645 (95%)	590 (96%)	21 (3%)	1 (0%)	47	57
1	L	608/645 (94%)	588 (97%)	20 (3%)	0	100	100
All	All	7328/7740 (95%)	7110 (97%)	217 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	590	GLU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	524/554 (95%)	522 (100%)	2 (0%)	91	94
1	B	530/554 (96%)	530 (100%)	0	100	100
1	C	530/554 (96%)	529 (100%)	1 (0%)	93	96
1	D	524/554 (95%)	523 (100%)	1 (0%)	93	96
1	E	530/554 (96%)	528 (100%)	2 (0%)	91	94
1	F	525/554 (95%)	522 (99%)	3 (1%)	86	91
1	G	526/554 (95%)	524 (100%)	2 (0%)	91	94
1	H	529/554 (96%)	528 (100%)	1 (0%)	93	96
1	I	530/554 (96%)	530 (100%)	0	100	100
1	J	525/554 (95%)	524 (100%)	1 (0%)	93	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	528/554 (95%)	525 (99%)	3 (1%)	86	91
1	L	525/554 (95%)	522 (99%)	3 (1%)	86	91
All	All	6326/6648 (95%)	6307 (100%)	19 (0%)	92	95

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	MET
1	A	193	ASN
1	C	68	MET
1	D	502	PHE
1	E	5	PHE
1	E	318	GLN
1	F	15	ASP
1	F	68	MET
1	F	463	GLN
1	G	68	MET
1	G	619	LEU
1	H	68	MET
1	J	180	PRO
1	K	193	ASN
1	K	215	ASP
1	K	589	ARG
1	L	68	MET
1	L	492	ASP
1	L	502	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	193	ASN
1	B	513	GLN
1	C	193	ASN
1	D	342	GLN
1	F	81	ASN
1	F	318	GLN
1	H	513	GLN
1	L	193	ASN
1	L	318	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	609/645 (94%)	-0.18	1 (0%) 95 95	24, 39, 59, 72	0
1	B	616/645 (95%)	-0.18	3 (0%) 91 91	24, 39, 62, 93	0
1	C	616/645 (95%)	-0.16	9 (1%) 73 71	26, 40, 67, 112	0
1	D	609/645 (94%)	-0.14	4 (0%) 87 87	27, 40, 61, 84	0
1	E	616/645 (95%)	-0.12	11 (1%) 68 64	29, 42, 72, 120	0
1	F	610/645 (94%)	-0.07	7 (1%) 80 79	24, 39, 66, 127	0
1	G	611/645 (94%)	-0.10	3 (0%) 91 91	26, 41, 63, 93	0
1	H	615/645 (95%)	-0.16	5 (0%) 86 85	23, 40, 65, 98	0
1	I	616/645 (95%)	-0.07	13 (2%) 63 60	29, 46, 70, 123	0
1	J	610/645 (94%)	-0.17	5 (0%) 86 85	25, 39, 65, 85	0
1	K	614/645 (95%)	-0.17	6 (0%) 82 81	29, 43, 72, 106	0
1	L	610/645 (94%)	-0.10	3 (0%) 91 91	26, 41, 65, 117	0
2	M	0/21	-	-	-	-
2	N	0/21	-	-	-	-
2	O	0/21	-	-	-	-
2	P	0/21	-	-	-	-
2	Q	0/21	-	-	-	-
2	R	0/21	-	-	-	-
2	S	0/21	-	-	-	-
2	T	0/21	-	-	-	-
2	U	0/21	-	-	-	-
2	V	0/21	-	-	-	-
2	W	0/21	-	-	-	-
2	X	0/21	-	-	-	-
All	All	7352/7992 (91%)	-0.13	70 (0%) 82 81	23, 41, 65, 127	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	588	ALA	8.0
1	I	587	ARG	6.1
1	C	587	ARG	6.1
1	H	362	LEU	4.5
1	C	588	ALA	4.3
1	C	584	ASN	4.2
1	E	585	ILE	4.1
1	K	619	LEU	3.9
1	F	587	ARG	3.9
1	E	589	ARG	3.7
1	E	587	ARG	3.6
1	I	589	ARG	3.6
1	E	588	ALA	3.6
1	K	589	ARG	3.5
1	C	589	ARG	3.3
1	F	494	VAL	3.2
1	I	585	ILE	3.2
1	C	352	GLY	3.1
1	E	4	VAL	3.1
1	I	352	GLY	3.0
1	J	353	ALA	2.9
1	K	588	ALA	2.8
1	I	408	TYR	2.8
1	K	587	ARG	2.7
1	C	408	TYR	2.6
1	E	416	LEU	2.6
1	L	493	THR	2.6
1	F	348	LEU	2.6
1	I	584	ASN	2.6
1	C	353	ALA	2.5
1	J	490	ILE	2.5
1	G	488	VAL	2.5
1	F	588	ALA	2.5
1	A	16	ARG	2.5
1	I	440	LYS	2.4
1	H	497	VAL	2.4
1	B	493	THR	2.4
1	J	348	LEU	2.4
1	I	620	ILE	2.3
1	C	585	ILE	2.3
1	D	364	THR	2.3
1	D	348	LEU	2.3
1	E	531	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	8	ILE	2.3
1	E	491	ASP	2.3
1	K	585	ILE	2.3
1	D	315	PRO	2.3
1	D	351	THR	2.3
1	H	493	THR	2.3
1	I	6	LYS	2.2
1	E	533	ILE	2.2
1	B	362	LEU	2.2
1	I	351	THR	2.2
1	F	589	ARG	2.2
1	I	590	GLU	2.2
1	G	31	ILE	2.2
1	L	438	GLN	2.1
1	H	353	ALA	2.1
1	B	500	THR	2.1
1	I	353	ALA	2.1
1	F	167	ALA	2.1
1	F	493	THR	2.1
1	C	197	LEU	2.1
1	E	619	LEU	2.1
1	E	80	GLY	2.1
1	G	127	ALA	2.1
1	L	531	HIS	2.1
1	K	80	GLY	2.1
1	J	350	THR	2.0
1	J	501	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.