



wwPDB EM Map/Model Validation Report ⓘ

Oct 24, 2016 – 02:21 PM EDT

PDB ID : 3JB1
EMDB ID: : EMD-6375
Title : Atomic model of cytoplasmic polyhedrosis virus with SAM
Authors : Yu, X.K.; Jiang, J.S.; Sun, J.C.; Zhou, Z.H.
Deposited on : 2015-07-06
Resolution : 3.10 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027939

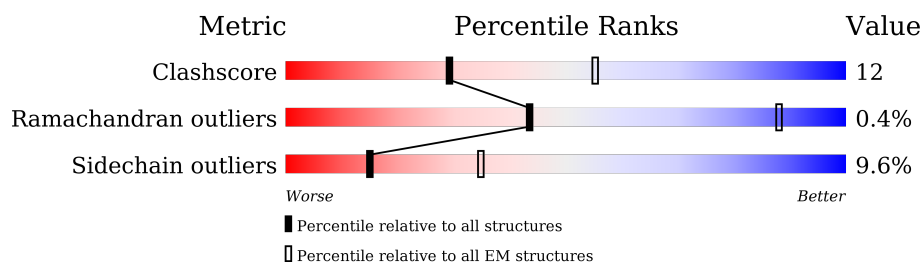
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	1058	
2	B	1333	
2	C	1333	
3	D	448	
3	E	448	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 32271 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Structural protein VP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1057	Total	C	N	O	S	0	0
			8434	5345	1457	1587	45		

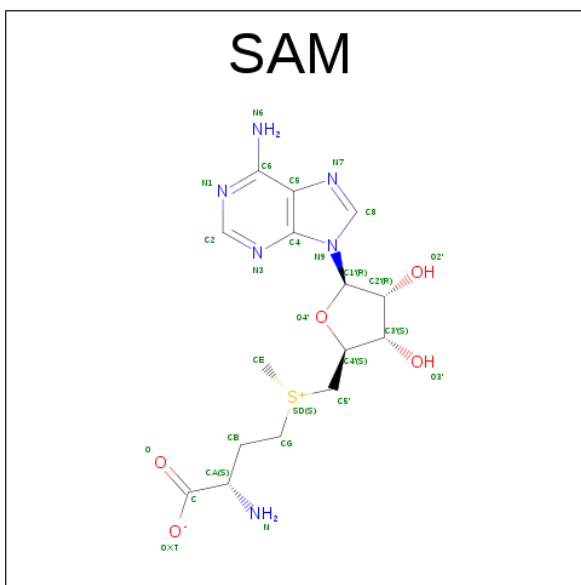
- Molecule 2 is a protein called Capsid protein VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1191	Total	C	N	O	S	0	0
			9397	5937	1634	1789	37		
2	C	1250	Total	C	N	O	S	0	0
			9851	6219	1712	1882	38		

- Molecule 3 is a protein called Viral structural protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	292	Total	C	N	O	S	0	0
			2281	1449	399	425	8		
3	E	292	Total	C	N	O	S	0	0
			2281	1449	399	425	8		

- Molecule 4 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula: C₁₅H₂₂N₆O₅S).

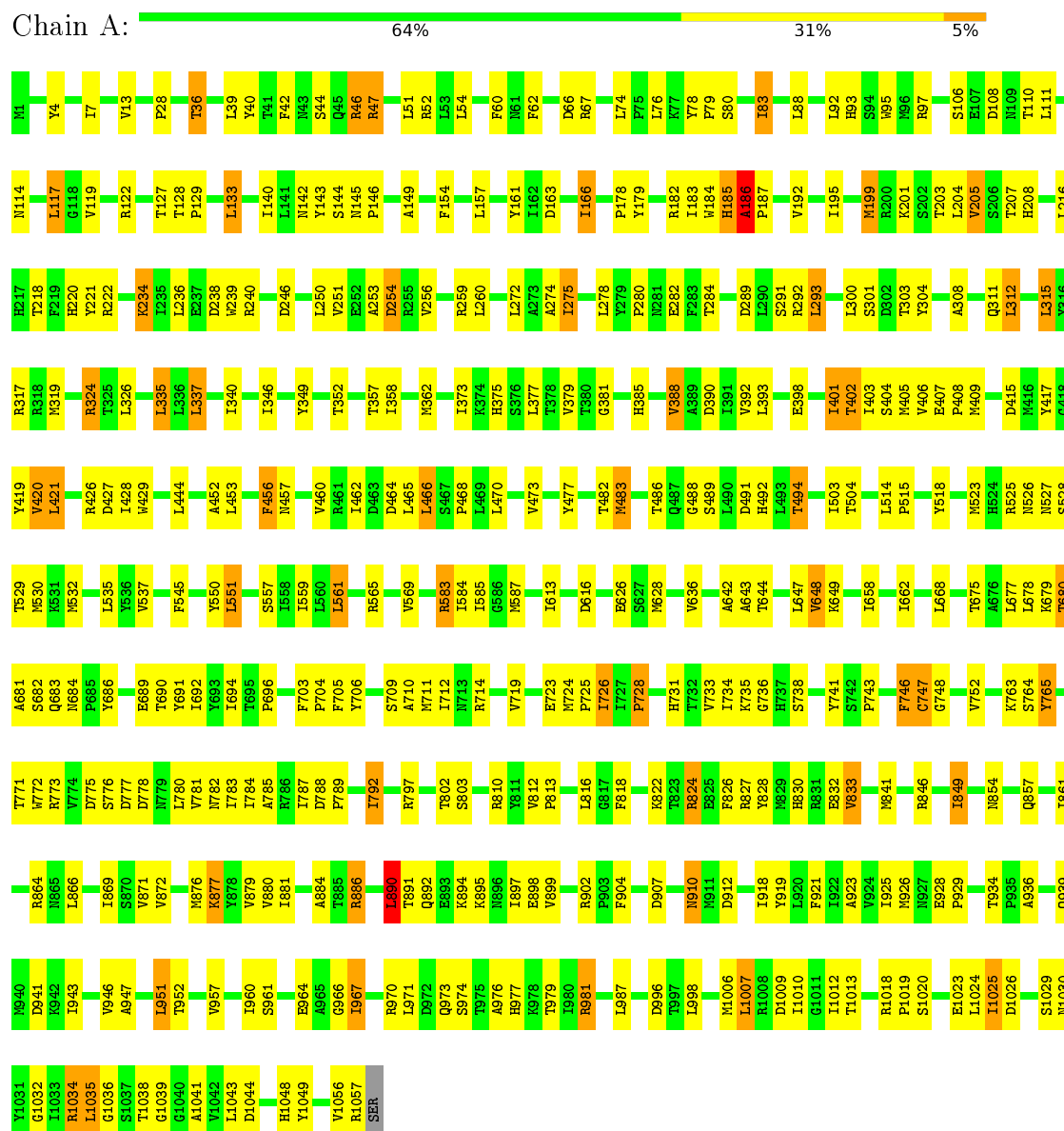


Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	S	0
			27	15	6	5	1	

3 Residue-property plots

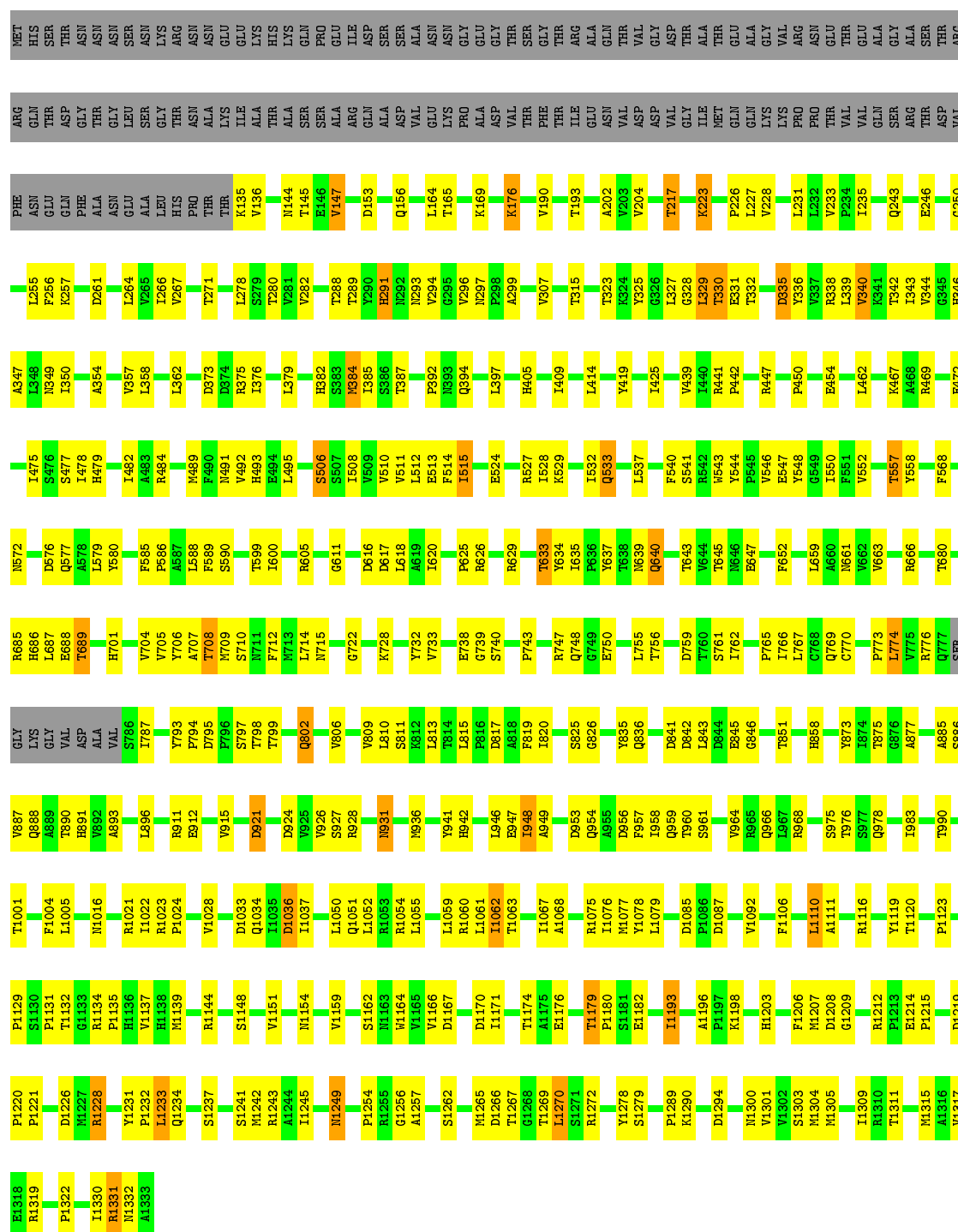
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric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

• Molecule 1: Structural protein VP3



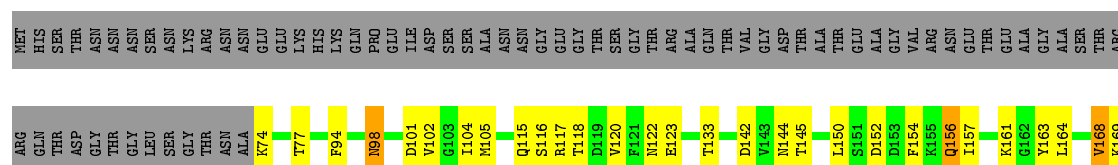
• Molecule 2: Capsid protein VP1





• Molecule 2: Capsid protein VP1

Chain C: 64% 26% 6%



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

VAL
ASP
GLU
ASN
GLU
TYR
GLY
ASN
SER
VAL
SER
GLU
LEU
THR
ILE
ASP
THR
GLN
SER
ASP
SER
VAL
LEU

● Molecule 3: Viral structural protein 5



M1
L2
Q3
Q4
I19
D22
T29
Q30
F31
L35
A39
L44
V45
T48
E53
T54
H55
L56
V66
D70
Q74
A81
F90
S91
R92
L93
L96
T101
L105
I111
Y112
M113
T116
D123
P124
T133
Y134
A135
K136
L137

G138
H139
D148
D151
H152
Y153
A154
H155
V156
E159
L160
D164
R167
V171
H172
P173
A177
D180
S181
W182
S185
L186
L189
S190
V193
W196
L199
D204
L213
R225
M226
R227
L228
F229
I230
T233
V240
R247
R250
V251

L252
E253
Y254
G256
V257
T262
T266
D272
L273
S274
R275
K281
F282
L283
T286
A292
ALA
SER
MET
ASP
ALA
ALA
MET
ILE
GLY
ARG
SER
MET
PRO
ASP
MET
HIS
VAL
GLU
THR
ARG
GLU
THR
THR
ASN
ILE
LYS
MET
PRO
ALA
GLY
ASN
GLU
ILE
ASP
ASN
M226
ALA
LEU
VAL
THR
ARG
HIS
ASN
ARG
TYR
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THR
GLU
PHE
ALA
GLU

LYS
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ASP
VAL
ASP
GLU
ASN
GLU
TYR
GLY
ASN
SER
VAL
SER
GLU
LEU
THR
ILE
ASP
THR
GLN
TRP
SER
ASP
SER
VAL
LEU

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	44908	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	59000	Depositor
Image detector	KODAK SO-163 FILM	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SAM

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 2$	RMSZ	# $ Z > 2$
1	A	0.28	0/8619	0.52	3/11737 (0.0%)
2	B	0.33	0/9590	0.54	0/13056
2	C	0.34	0/10052	0.56	0/13687
3	D	0.33	0/2327	0.54	0/3163
3	E	0.30	0/2327	0.52	0/3163
All	All	0.32	0/32915	0.54	3/44806 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	186	ALA	C-N-CD	-8.20	102.57	120.60
1	A	186	ALA	C-N-CA	5.69	145.91	122.00
1	A	890	LEU	CA-CB-CG	5.39	127.70	115.30

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	8434	0	8399	219	0
2	B	9397	0	9315	255	0
2	C	9851	0	9762	224	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	2281	0	2282	62	0
3	E	2281	0	2282	47	0
4	A	27	0	22	5	0
All	All	32271	0	32062	785	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 12.

All (785) 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)
2:C:709:MET:O	2:C:715:ASN:ND2	2.09	0.85
2:C:873:TYR:HB3	2:C:898:GLN:HB2	1.60	0.83
3:D:44:LEU:HG	3:D:174:VAL:HG22	1.64	0.79
1:A:752:VAL:HG12	1:A:781:VAL:HG23	1.65	0.78
2:C:462:LEU:HD13	2:C:680:THR:HG22	1.64	0.78
2:B:891:HIS:HA	3:D:242:ARG:HD3	1.67	0.76
2:B:1134:ARG:NH1	2:B:1154:ASN:OD1	2.16	0.76
2:C:1208:ASP:OD2	2:C:1243:ARG:NH2	2.20	0.75
2:B:228:VAL:HG23	2:B:250:GLY:HA2	1.68	0.74
1:A:111:LEU:HD13	1:A:142:ASN:HB3	1.70	0.74
2:C:307:VAL:HG21	2:C:1245:ILE:HG22	1.69	0.74
3:E:233:THR:HG22	3:E:252:LEU:HD13	1.70	0.74
2:C:350:ILE:O	2:C:1300:ASN:ND2	2.21	0.74
2:C:1144:ARG:NH2	2:C:1196:ALA:O	2.21	0.73
3:D:164:ASP:OD2	3:D:167:ARG:NH2	2.21	0.73
2:C:333:ARG:NH1	3:E:22:ASP:OD1	2.22	0.72
2:B:339:LEU:HD21	3:D:63:PRO:HB2	1.71	0.72
2:C:1254:PRO:HG2	2:C:1257:ALA:HB2	1.71	0.72
1:A:773:ARG:NH2	1:A:778:ASP:O	2.22	0.72
1:A:680:THR:HG23	1:A:683:GLN:HB2	1.71	0.72
2:C:332:THR:HG22	2:C:334:LEU:H	1.54	0.71
2:B:739:GLY:HA2	2:C:653:ARG:HD3	1.73	0.71
1:A:583:ARG:H	1:A:583:ARG:HH11	1.39	0.70
3:D:85:ASN:HB3	3:D:141:SER:HB3	1.72	0.70
2:B:576:ASP:H	2:B:579:LEU:HD12	1.56	0.70
2:C:704:VAL:HB	2:C:1330:ILE:HD11	1.74	0.70
1:A:857:GLN:OE1	1:A:877:LYS:NZ	2.24	0.70
2:C:674:LYS:HE3	2:C:677:ARG:HE	1.58	0.69
2:B:629:ARG:NH1	2:B:1036:ASP:O	2.25	0.69
2:B:704:VAL:HA	2:B:1330:ILE:HD11	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:491:ASN:ND2	2:B:750:GLU:O	2.26	0.69
2:B:921:ASP:OD1	2:B:928:ARG:NH2	2.22	0.69
2:C:469:ARG:NH2	2:C:513:GLU:OE2	2.26	0.68
2:B:350:ILE:O	2:B:1300:ASN:ND2	2.26	0.68
3:E:81:ALA:HB3	3:E:275:ARG:HD3	1.76	0.68
2:B:1171:ILE:HD13	2:B:1193:ILE:HD12	1.74	0.68
3:E:56:LEU:HD22	3:E:135:ALA:HB3	1.76	0.68
2:B:795:ASP:OD2	2:B:1319:ARG:NH1	2.26	0.67
1:A:127:THR:HG21	2:B:640:GLN:HA	1.77	0.67
2:C:461:ARG:HB3	2:C:676:THR:HG21	1.75	0.67
2:C:244:SER:HA	2:C:1201:LEU:HD22	1.75	0.67
2:C:313:ASP:OD1	2:C:1253:ARG:NH2	2.27	0.67
1:A:880:VAL:HB	1:A:899:VAL:HG13	1.77	0.67
2:C:772:TYR:HB2	2:C:775:VAL:HG23	1.76	0.66
1:A:407:GLU:O	1:A:1034:ARG:NH1	2.28	0.66
3:E:164:ASP:OD1	3:E:167:ARG:NH2	2.29	0.66
2:C:183:SER:OG	2:C:186:ASP:OD2	2.14	0.66
1:A:393:LEU:HB3	1:A:748:GLY:HA3	1.77	0.66
2:B:954:GLN:HG2	3:D:240:VAL:HG12	1.77	0.65
2:B:376:ILE:HD11	2:B:1317:VAL:HG11	1.79	0.65
1:A:192:VAL:HG22	1:A:216:LEU:HD22	1.78	0.65
1:A:735:LYS:O	1:A:765:TYR:OH	2.14	0.65
2:B:484:ARG:O	2:B:527:ARG:NH2	2.29	0.65
1:A:203:THR:HG22	1:A:204:LEU:HG	1.77	0.65
1:A:559:ILE:HG22	1:A:585:ILE:HB	1.76	0.65
2:B:1078:TYR:OH	2:C:123:GLU:OE1	2.15	0.65
3:E:272:ASP:OD2	3:E:274:SER:OG	2.12	0.65
2:B:442:PRO:HB3	2:B:475:ILE:HG21	1.77	0.65
1:A:178:PRO:HB2	1:A:179:TYR:HD2	1.61	0.65
3:D:19:ILE:HD11	3:D:31:PHE:HB2	1.79	0.64
1:A:861:ILE:HG13	1:A:881:ILE:HB	1.78	0.64
3:D:46:LYS:HD3	3:D:158:LEU:HD23	1.79	0.64
1:A:254:ASP:OD1	1:A:254:ASP:N	2.30	0.64
1:A:532:MET:HA	1:A:535:LEU:HD12	1.79	0.64
3:E:105:LEU:HD21	3:E:199:LEU:HD13	1.78	0.64
2:B:1208:ASP:OD1	2:B:1243:ARG:NH2	2.21	0.64
2:C:1060:ARG:NH1	2:C:1291:LEU:O	2.29	0.63
3:D:107:LEU:HD22	3:D:120:PRO:HB2	1.81	0.63
1:A:462:ILE:HG13	1:A:466:LEU:HD22	1.80	0.63
2:C:921:ASP:OD1	2:C:928:ARG:NH2	2.25	0.63
1:A:427:ASP:HA	1:A:703:PHE:HA	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:733:VAL:HG12	2:C:743:PRO:HA	1.82	0.62
2:B:626:ARG:NH2	2:B:712:PHE:O	2.33	0.62
1:A:66:ASP:HB3	1:A:95:TRP:HE1	1.64	0.62
2:B:893:ALA:HB1	2:B:915:VAL:HA	1.81	0.62
2:B:1144:ARG:NH2	2:B:1196:ALA:O	2.33	0.62
2:C:1305:MET:HE2	2:C:1309:ILE:HD11	1.80	0.62
2:B:750:GLU:OE1	2:C:452:ASN:ND2	2.31	0.62
1:A:1020:SER:OG	1:A:1023:GLU:OE2	2.16	0.62
2:B:325:TYR:OH	2:B:349:ASN:OD1	2.14	0.62
2:B:956:ASP:OD2	3:D:266:THR:OG1	2.18	0.62
2:C:163:TYR:N	2:C:351:ASP:OD1	2.32	0.62
1:A:426:ARG:NH1	1:A:428:ILE:O	2.32	0.62
1:A:514:LEU:HD12	1:A:515:PRO:HD2	1.82	0.62
1:A:236:LEU:HD13	1:A:293:LEU:HD21	1.81	0.62
1:A:690:THR:HG21	1:A:711:MET:HB3	1.82	0.62
2:B:450:PRO:HG3	2:B:686:HIS:HB2	1.82	0.62
2:C:841:ASP:OD2	2:C:911:ARG:NH2	2.33	0.61
2:B:1272:ARG:HD3	3:D:70:ASP:HA	1.82	0.61
1:A:879:VAL:HG22	1:A:898:GLU:HB3	1.81	0.61
1:A:797:ARG:NH2	1:A:876:MET:O	2.30	0.61
3:D:2:LEU:HD12	3:D:107:LEU:HD21	1.82	0.61
1:A:178:PRO:HB2	1:A:179:TYR:CD2	2.36	0.61
2:C:370:VAL:HG12	2:C:398:ARG:HB2	1.83	0.61
2:C:713:MET:HG2	2:C:714:LEU:HG	1.83	0.61
2:B:961:SER:HB3	2:B:964:VAL:HG23	1.82	0.61
1:A:477:TYR:HA	1:A:482:THR:HG22	1.83	0.61
1:A:613:ILE:HG13	1:A:643:ALA:HB2	1.83	0.60
2:B:1085:ASP:OD2	2:B:1243:ARG:NH2	2.27	0.60
2:C:299:ALA:HB2	2:C:1265:MET:HB3	1.83	0.60
2:B:776:ARG:HD3	2:B:787:ILE:HB	1.81	0.60
2:C:341:LYS:HD2	2:C:1307:ALA:HB3	1.84	0.60
1:A:326:LEU:HB3	1:A:352:THR:HG22	1.83	0.60
2:C:712:PHE:HB2	2:C:715:ASN:ND2	2.15	0.60
2:B:1226:ASP:OD2	2:C:122:ASN:ND2	2.33	0.60
2:B:256:PHE:HE2	2:B:990:THR:HG21	1.67	0.60
2:B:733:VAL:HG12	2:B:743:PRO:HA	1.83	0.59
2:C:382:HIS:ND1	2:C:799:THR:HG23	2.17	0.59
1:A:385:HIS:NE2	1:A:803:SER:OG	2.34	0.59
2:C:817:ASP:O	2:C:821:ASN:ND2	2.27	0.59
2:C:980:ARG:NH2	2:C:997:TYR:O	2.35	0.59
2:B:841:ASP:OD1	2:B:911:ARG:NH2	2.26	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:LEU:HD21	1:A:530:MET:HE2	1.84	0.59
2:B:953:ASP:HB3	3:D:241:ASN:HB2	1.83	0.59
1:A:828:TYR:HB3	1:A:1034:ARG:HB3	1.84	0.59
2:B:153:ASP:N	2:B:153:ASP:OD1	2.35	0.59
2:C:838:GLU:OE1	2:C:933:ASN:ND2	2.36	0.59
1:A:565:ARG:NH2	1:A:616:ASP:OD2	2.35	0.59
2:C:748:GLN:HG3	2:C:1000:LEU:HD22	1.85	0.59
2:C:1211:LEU:HD21	2:C:1246:VAL:HG21	1.84	0.59
1:A:957:VAL:HG22	1:A:1056:VAL:HG23	1.84	0.59
2:B:817:ASP:HA	2:B:983:ILE:HG12	1.85	0.59
1:A:208:HIS:HE1	1:A:234:LYS:HG2	1.68	0.58
2:B:1266:ASP:OD2	2:B:1279:SER:N	2.29	0.58
1:A:409:MET:HE2	1:A:465:LEU:HD22	1.85	0.58
2:B:439:VAL:HG11	2:B:705:VAL:HG21	1.85	0.58
2:B:256:PHE:CE2	2:B:990:THR:HG21	2.38	0.58
2:B:329:LEU:HB2	2:B:346:HIS:CE1	2.37	0.58
2:C:776:ARG:HB3	2:C:787:ILE:HD12	1.84	0.58
2:C:833:ARG:HG3	2:C:922:TYR:CZ	2.37	0.58
1:A:686:TYR:CZ	1:A:1035:LEU:HB2	2.39	0.58
1:A:923:ALA:N	1:A:961:SER:OG	2.35	0.58
2:B:1228:ARG:HG2	2:B:1231:TYR:CZ	2.39	0.58
2:C:115:GLN:HB3	2:C:117:ARG:HD3	1.84	0.58
1:A:833:VAL:HG12	1:A:1043:LEU:HD23	1.86	0.58
2:C:410:ARG:HD3	2:C:1043:SER:HA	1.85	0.58
3:D:233:THR:HG22	3:D:252:LEU:HD13	1.86	0.58
1:A:129:PRO:HD2	2:B:1332:ASN:HB2	1.84	0.58
1:A:78:TYR:HE1	1:A:83:ILE:HG23	1.69	0.57
2:B:806:VAL:HG22	2:B:1001:THR:HG21	1.85	0.57
2:B:384:MET:HA	2:B:708:THR:HG21	1.86	0.57
2:B:462:LEU:HD13	2:B:680:THR:HG22	1.86	0.57
2:C:503:GLU:OE2	2:C:542:ARG:NH2	2.32	0.57
3:D:56:LEU:HD22	3:D:135:ALA:HB3	1.87	0.57
1:A:951:LEU:HD13	1:A:1057:ARG:HH12	1.69	0.57
2:C:414:LEU:HD23	2:C:814:THR:HB	1.87	0.57
2:C:504:ASP:OD2	2:C:506:SER:OG	2.23	0.57
2:C:450:PRO:HG3	2:C:686:HIS:HB2	1.87	0.57
2:B:1331:ARG:HB3	2:B:1331:ARG:HH11	1.69	0.57
2:B:558:TYR:CZ	2:B:585:PHE:HB2	2.39	0.57
1:A:163:ASP:OD1	1:A:182:ARG:NE	2.33	0.57
2:B:335:ASP:OD2	2:B:340:VAL:N	2.38	0.56
1:A:317:ARG:NH1	3:D:41:GLU:OE1	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:LEU:HD11	1:A:973:GLN:HB2	1.87	0.56
1:A:420:VAL:HA	1:A:974:SER:HB2	1.88	0.56
2:C:1023:ARG:HB3	2:C:1025:ASP:OD1	2.06	0.56
2:C:1214:GLU:HG2	2:C:1215:PRO:HD2	1.86	0.56
2:B:1131:PRO:O	2:B:1162:SER:OG	2.14	0.56
3:D:233:THR:HB	3:D:268:THR:HG21	1.86	0.56
1:A:275:ILE:HG13	1:A:301:SER:HA	1.88	0.56
1:A:775:ASP:OD1	1:A:776:SER:N	2.38	0.56
2:B:328:GLY:HA3	2:B:347:ALA:H	1.71	0.56
2:B:479:HIS:HA	2:B:482:ILE:HD12	1.87	0.56
1:A:1026:ASP:OD1	1:A:1030:ASN:ND2	2.39	0.55
2:C:161:LYS:HD2	2:C:212:PHE:HB2	1.88	0.55
2:C:887:VAL:HG22	2:C:893:ALA:HA	1.89	0.55
1:A:373:ILE:HG21	1:A:375:HIS:CE1	2.41	0.55
1:A:846:ARG:HB2	1:A:871:VAL:HA	1.89	0.55
1:A:526:ASN:OD1	1:A:529:THR:OG1	2.17	0.55
2:C:169:LYS:HB2	2:C:203:VAL:HG23	1.87	0.55
2:C:576:ASP:OD1	2:C:747:ARG:NH2	2.40	0.55
1:A:904:PHE:H	4:A:1101:SAM:H2	1.71	0.55
2:B:439:VAL:HG12	2:B:701:HIS:NE2	2.22	0.55
2:B:958:ILE:HG22	2:B:960:THR:HG23	1.88	0.55
3:E:4:GLN:NE2	3:E:204:ASP:OD2	2.39	0.55
1:A:274:ALA:HA	1:A:319:MET:HE2	1.89	0.55
2:B:1051:GLN:O	2:B:1055:LEU:HB2	2.06	0.55
2:C:1013:LYS:HE2	2:C:1015:GLN:NE2	2.21	0.55
3:E:90:PHE:HA	3:E:93:LEU:HB2	1.87	0.55
1:A:144:SER:OG	1:A:145:ASN:N	2.40	0.55
3:E:66:VAL:HG13	3:E:111:ILE:HB	1.89	0.55
1:A:404:SER:HB2	1:A:826:PHE:HD1	1.72	0.54
2:B:643:THR:HG22	2:B:645:THR:H	1.72	0.54
2:B:1289:PRO:HG2	3:D:191:ARG:NH2	2.22	0.54
2:C:1002:LEU:HD12	2:C:1005:LEU:HB2	1.87	0.54
1:A:939:GLN:HB2	1:A:998:LEU:HD21	1.89	0.54
2:B:1111:ALA:HB3	2:B:1116:ARG:HD2	1.90	0.54
2:C:612:PHE:HZ	2:C:1330:ILE:HG22	1.71	0.54
2:C:611:GLY:HA3	2:C:635:ILE:O	2.08	0.54
2:C:949:ALA:HA	2:C:958:ILE:HD13	1.89	0.54
2:C:228:VAL:HG23	2:C:250:GLY:HA2	1.89	0.54
2:B:652:PHE:HE2	2:B:688:GLU:HA	1.72	0.54
1:A:488:GLY:H	1:A:492:HIS:HD1	1.55	0.54
2:B:1076:ILE:HG22	2:B:1159:VAL:HG11	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:261:ASP:HB3	2:B:357:VAL:HG11	1.90	0.54
2:B:397:LEU:HA	2:B:1309:ILE:HD13	1.89	0.54
1:A:525:ARG:HG2	1:A:529:THR:HG21	1.91	0.53
3:E:180:ASP:OD2	3:E:247:ARG:NH1	2.42	0.53
2:B:1249:ASN:N	2:B:1249:ASN:OD1	2.33	0.53
2:B:145:THR:HB	2:B:1317:VAL:HG23	1.90	0.53
2:C:612:PHE:CZ	2:C:1330:ILE:HG22	2.43	0.53
2:C:261:ASP:OD1	2:C:263:ARG:NH1	2.41	0.53
3:D:283:LEU:HA	3:D:286:THR:HG22	1.90	0.53
2:B:491:ASN:HD22	2:B:756:THR:HG21	1.74	0.53
2:B:409:ILE:HD13	2:B:625:PRO:HB2	1.89	0.53
1:A:569:VAL:HG13	1:A:584:ILE:HG22	1.89	0.53
2:C:294:VAL:HG11	2:C:327:LEU:HD21	1.91	0.53
2:C:450:PRO:HD2	2:C:453:LEU:HD22	1.91	0.53
1:A:528:SER:OG	1:A:565:ARG:NH1	2.41	0.53
3:D:108:ASP:OD1	3:D:112:TYR:OH	2.24	0.53
2:C:1114:ARG:HH21	2:C:1116:ARG:CZ	2.22	0.53
2:B:335:ASP:OD1	2:B:340:VAL:HG22	2.09	0.52
2:C:332:THR:HG23	2:C:1270:LEU:HD12	1.92	0.52
3:E:190:SER:HA	3:E:230:ILE:HD12	1.91	0.52
1:A:929:PRO:HA	4:A:1101:SAM:H2'	1.91	0.52
2:C:384:MET:HA	2:C:708:THR:HG21	1.91	0.52
2:C:448:TYR:CZ	2:C:470:ALA:HB1	2.44	0.52
2:B:425:ILE:HG13	2:B:1004:PHE:CD2	2.44	0.52
2:B:558:TYR:HB3	2:B:568:PHE:CD1	2.44	0.52
2:C:824:LEU:HD23	2:C:971:MET:HE1	1.91	0.52
1:A:406:VAL:HG11	1:A:460:VAL:HG13	1.90	0.52
1:A:40:TYR:HB2	1:A:51:LEU:HD13	1.90	0.52
1:A:689:GLU:N	1:A:689:GLU:OE1	2.42	0.52
1:A:704:PRO:HG2	1:A:705:PHE:CD2	2.45	0.52
2:C:734:ILE:HG22	2:C:1017:ALA:HB1	1.92	0.52
2:C:980:ARG:HB2	2:C:980:ARG:HH11	1.75	0.52
1:A:133:LEU:HD11	1:A:140:ILE:HD13	1.91	0.52
1:A:385:HIS:HB3	1:A:388:VAL:HG13	1.92	0.52
1:A:66:ASP:OD1	1:A:122:ARG:NH2	2.43	0.52
2:B:611:GLY:HA3	2:B:635:ILE:O	2.10	0.52
1:A:812:VAL:HG22	1:A:816:LEU:HD11	1.92	0.52
2:B:704:VAL:O	2:B:708:THR:HG23	2.09	0.52
2:B:826:GLY:HA3	2:B:949:ALA:HB2	1.91	0.52
2:C:213:PHE:HB3	2:C:219:ILE:HD12	1.90	0.52
3:E:177:ALA:HB3	3:E:252:LEU:HG	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:PRO:HB2	1:A:468:PRO:HG3	1.92	0.52
2:B:616:ASP:OD2	2:B:710:SER:OG	2.28	0.52
1:A:1039:GLY:O	1:A:1043:LEU:HB2	2.10	0.51
2:B:1036:ASP:OD1	2:B:1036:ASP:N	2.43	0.51
2:B:887:VAL:HG22	2:B:893:ALA:HA	1.91	0.51
2:C:104:ILE:HG12	2:C:1311:THR:HG23	1.92	0.51
2:C:1197:PRO:HG2	2:C:1200:LYS:HB2	1.92	0.51
2:C:962:ASP:N	2:C:962:ASP:OD1	2.42	0.51
1:A:675:THR:HG22	1:A:694:ILE:HG12	1.90	0.51
1:A:199:MET:HE3	1:A:220:HIS:HE1	1.75	0.51
1:A:964:GLU:HG3	1:A:966:GLY:H	1.75	0.51
2:B:469:ARG:NH1	2:B:472:GLU:OE1	2.43	0.51
2:C:161:LYS:O	2:C:263:ARG:NH2	2.43	0.51
3:E:92:ARG:NH2	3:E:113:ASN:HB2	2.25	0.51
1:A:13:VAL:HG21	1:A:146:PRO:HB3	1.93	0.51
1:A:649:LYS:HB2	1:A:691:TYR:CE1	2.44	0.51
2:B:1135:PRO:O	2:B:1137:VAL:HG23	2.10	0.51
2:B:975:SER:N	2:B:978:GLN:OE1	2.42	0.51
2:B:1180:PRO:HA	2:B:1207:MET:SD	2.51	0.51
2:B:342:THR:OG1	2:B:343:ILE:N	2.44	0.51
2:C:1077:MET:HG3	2:C:1165:VAL:HG22	1.91	0.51
1:A:771:THR:HG22	1:A:783:ILE:HG12	1.93	0.51
2:B:544:TYR:HB3	2:B:547:GLU:HB2	1.93	0.51
2:B:586:PRO:HB2	2:B:589:PHE:HD2	1.75	0.51
2:B:558:TYR:CE1	2:B:590:SER:HB3	2.46	0.51
2:C:204:VAL:HG11	2:C:1242:MET:HE2	1.92	0.51
1:A:527:ASN:HD21	1:A:684:ASN:HD21	1.58	0.51
1:A:557:SER:HB3	1:A:583:ARG:HB2	1.91	0.51
2:B:1179:THR:HG23	2:B:1182:GLU:HG2	1.92	0.51
2:B:533:GLN:HB2	2:B:588:LEU:HD12	1.92	0.51
2:C:606:LEU:HA	2:C:651:ARG:HH21	1.76	0.51
3:D:53:GLU:H	3:D:53:GLU:CD	2.14	0.51
2:B:469:ARG:NH2	2:B:513:GLU:OE2	2.43	0.51
2:C:228:VAL:HG21	2:C:253:MET:HG2	1.93	0.51
2:C:875:THR:OG1	2:C:876:GLY:N	2.43	0.51
3:D:112:TYR:CE2	3:D:119:ILE:HG21	2.46	0.51
3:D:53:GLU:OE2	3:D:281:LYS:NZ	2.27	0.51
1:A:420:VAL:HA	1:A:974:SER:CB	2.41	0.50
2:B:307:VAL:HG21	2:B:1245:ILE:HG22	1.93	0.50
1:A:420:VAL:HG13	1:A:976:ALA:HB3	1.91	0.50
2:B:825:SER:HB2	2:B:1016:ASN:HD21	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:585:PHE:CE1	2:B:728:LYS:HE2	2.46	0.50
2:C:1118:THR:HA	2:C:1129:PRO:HA	1.92	0.50
2:C:528:ILE:HG13	2:C:532:ILE:HD12	1.93	0.50
2:C:533:GLN:HG3	2:C:588:LEU:HD12	1.92	0.50
2:C:799:THR:HA	2:C:802:GLN:HG2	1.92	0.50
1:A:280:PRO:HB3	1:A:304:TYR:CE1	2.46	0.50
3:D:79:ILE:HA	3:D:269:ILE:HG22	1.92	0.50
2:B:1062:ILE:HG22	2:B:1063:THR:HG23	1.92	0.50
2:C:357:VAL:HG23	2:C:1057:VAL:HG11	1.94	0.50
3:E:182:TRP:NE1	3:E:185:SER:HA	2.26	0.50
1:A:381:GLY:H	1:A:802:THR:HB	1.76	0.50
2:B:1144:ARG:NH1	2:B:1170:ASP:OD2	2.44	0.50
2:B:1254:PRO:HG2	2:B:1257:ALA:HB2	1.94	0.50
2:B:156:GLN:HB3	2:B:266:ILE:HD11	1.93	0.50
2:B:441:ARG:HH22	2:B:773:PRO:HB3	1.77	0.50
2:C:334:LEU:HD22	2:C:337:VAL:HG21	1.92	0.50
2:C:616:ASP:OD1	2:C:710:SER:OG	2.25	0.50
1:A:239:TRP:CZ2	1:A:280:PRO:HD2	2.46	0.50
1:A:452:ALA:HB2	1:A:725:PRO:HB3	1.94	0.50
2:B:299:ALA:HB2	2:B:1265:MET:HB3	1.93	0.50
2:C:390:HIS:HB2	2:C:1318:GLU:HB3	1.94	0.50
3:E:45:VAL:HG13	3:E:171:VAL:HG12	1.94	0.50
1:A:830:HIS:HB2	1:A:1034:ARG:NH1	2.27	0.49
1:A:402:THR:HG23	1:A:824:ARG:HB3	1.94	0.49
1:A:417:TYR:HB3	1:A:537:VAL:HG11	1.94	0.49
1:A:726:ILE:HG13	1:A:1029:SER:HB2	1.94	0.49
2:B:204:VAL:HB	2:B:1242:MET:HB2	1.94	0.49
2:C:504:ASP:OD1	2:C:504:ASP:N	2.44	0.49
3:D:253:GLU:HB2	3:D:254:TYR:CD1	2.46	0.49
2:B:508:ILE:HG21	2:B:663:VAL:HG21	1.93	0.49
1:A:907:ASP:HB2	1:A:910:ASN:HD21	1.77	0.49
2:B:1206:PHE:CE1	2:B:1232:PRO:HD3	2.48	0.49
2:C:1243:ARG:HD3	2:C:1256:GLY:O	2.12	0.49
1:A:303:THR:HG21	1:A:813:PRO:HD3	1.94	0.49
2:B:169:LYS:NZ	2:B:1182:GLU:OE2	2.37	0.49
2:C:323:THR:HG21	2:C:1262:SER:HB2	1.93	0.49
3:D:186:LEU:HD22	3:D:233:THR:HG21	1.93	0.49
1:A:636:VAL:HG22	1:A:648:VAL:HG11	1.95	0.49
2:C:1080:THR:OG1	2:C:1082:ASP:OD1	2.29	0.49
3:E:283:LEU:HA	3:E:286:THR:HG22	1.95	0.49
1:A:892:GLN:HA	1:A:897:ILE:HB	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1023:ARG:HG2	2:B:1024:PRO:HD2	1.94	0.49
1:A:60:PHE:HA	1:A:119:VAL:HG11	1.95	0.49
1:A:457:ASN:HA	1:A:686:TYR:HB2	1.93	0.49
2:B:1266:ASP:OD1	2:B:1279:SER:OG	2.24	0.49
2:B:921:ASP:N	2:B:921:ASP:OD1	2.44	0.49
2:C:206:ILE:HD13	2:C:1298:PHE:HE2	1.77	0.49
3:D:105:LEU:HD21	3:D:199:LEU:HD13	1.94	0.49
1:A:377:LEU:H	1:A:377:LEU:HD12	1.77	0.49
1:A:773:ARG:HG2	1:A:781:VAL:HG22	1.94	0.49
1:A:292:ARG:NH2	1:A:777:ASP:OD1	2.46	0.49
2:B:338:ARG:HH11	2:B:397:LEU:HD23	1.77	0.49
2:C:1106:PHE:CE1	2:C:1119:TYR:HB2	2.48	0.49
2:C:828:ASP:N	2:C:828:ASP:OD2	2.46	0.49
1:A:404:SER:HB2	1:A:826:PHE:CD1	2.48	0.49
1:A:488:GLY:HA2	1:A:551:LEU:HD13	1.94	0.49
2:B:1129:PRO:HD3	3:E:273:LEU:HD23	1.95	0.49
2:C:606:LEU:HD22	2:C:655:ILE:HG12	1.94	0.49
2:C:980:ARG:NH1	2:C:980:ARG:HB2	2.28	0.49
2:C:865:ILE:HD11	2:C:1041:ARG:O	2.12	0.48
2:B:484:ARG:NE	2:B:524:GLU:OE2	2.46	0.48
2:B:712:PHE:HB2	2:B:715:ASN:OD1	2.13	0.48
2:B:193:THR:HG21	2:B:297:ASN:O	2.13	0.48
2:B:373:ASP:HA	2:B:1315:MET:HE1	1.94	0.48
2:B:957:PHE:CE1	2:B:1016:ASN:HB3	2.48	0.48
2:C:388:GLN:HB3	2:C:1320:VAL:HG13	1.96	0.48
1:A:947:ALA:HB3	1:A:1010:ILE:HD13	1.95	0.48
2:B:1110:LEU:HD13	3:E:272:ASP:HB3	1.94	0.48
2:B:1144:ARG:HH11	2:B:1170:ASP:HB3	1.78	0.48
2:C:326:GLY:H	2:C:1267:THR:HG21	1.77	0.48
3:E:186:LEU:HD22	3:E:233:THR:HG21	1.94	0.48
1:A:967:ILE:HB	1:A:1049:TYR:HB3	1.95	0.48
2:B:387:THR:HG22	2:B:1322:PRO:HD3	1.95	0.48
2:C:223:LYS:NZ	2:C:1203:HIS:HB2	2.28	0.48
1:A:392:VAL:HG22	1:A:733:VAL:HG12	1.95	0.48
2:B:558:TYR:CE1	2:B:585:PHE:HB2	2.48	0.48
2:C:302:ARG:HD2	2:C:318:LEU:HD12	1.95	0.48
2:B:634:TYR:CE1	2:B:722:GLY:HA3	2.49	0.48
1:A:199:MET:CE	1:A:220:HIS:HE1	2.26	0.48
2:B:732:TYR:CE1	2:B:1021:ARG:HG2	2.49	0.48
2:C:613:LEU:HD11	2:C:632:GLN:HB3	1.96	0.48
1:A:154:PHE:CD2	1:A:185:HIS:HA	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:TYR:OH	1:A:246:ASP:OD1	2.23	0.48
1:A:746:PHE:CE2	1:A:787:ILE:HD11	2.49	0.48
1:A:879:VAL:HA	1:A:898:GLU:O	2.14	0.48
2:C:1241:SER:OG	2:C:1264:GLU:OE2	2.25	0.48
1:A:1026:ASP:O	1:A:1030:ASN:ND2	2.32	0.48
1:A:201:LYS:O	2:B:629:ARG:HG2	2.14	0.48
1:A:462:ILE:HA	1:A:465:LEU:HD12	1.96	0.48
1:A:919:TYR:HB3	1:A:921:PHE:CE2	2.49	0.48
2:C:683:TRP:CZ2	2:C:687:LEU:HD11	2.49	0.48
1:A:822:LYS:HE2	1:A:822:LYS:HB3	1.69	0.47
2:B:776:ARG:HB3	2:B:787:ILE:H	1.79	0.47
2:C:493:HIS:HB3	2:C:758:ILE:HD13	1.96	0.47
2:C:813:LEU:HA	2:C:992:VAL:HG11	1.95	0.47
2:C:970:LEU:HD23	2:C:970:LEU:HA	1.72	0.47
3:E:39:ALA:HB1	3:E:173:PRO:HB2	1.96	0.47
2:B:1106:PHE:CE1	2:B:1119:TYR:HB2	2.49	0.47
2:B:217:THR:HG23	2:B:257:LYS:HD3	1.96	0.47
2:C:190:VAL:O	2:C:194:VAL:HG23	2.13	0.47
2:C:494:GLU:HB2	2:C:757:ILE:HD13	1.96	0.47
3:D:68:ILE:HD11	3:D:90:PHE:HA	1.96	0.47
3:E:53:GLU:OE1	3:E:281:LYS:NZ	2.47	0.47
1:A:489:SER:OG	1:A:491:ASP:OD2	2.32	0.47
1:A:709:SER:HB2	1:A:712:ILE:HG13	1.96	0.47
2:B:1087:ASP:OD2	2:B:1237:SER:OG	2.32	0.47
2:B:327:LEU:HA	2:B:327:LEU:HD12	1.68	0.47
2:B:392:PRO:HG2	2:B:394:GLN:HG3	1.96	0.47
2:B:633:THR:HG21	2:B:710:SER:HB2	1.95	0.47
2:B:419:TYR:HB3	2:B:1005:LEU:HD22	1.95	0.47
2:B:552:VAL:HG22	2:B:572:ASN:HB2	1.96	0.47
2:C:999:LYS:HG2	2:C:1009:THR:HA	1.96	0.47
2:C:1031:TYR:OH	2:C:1038:GLU:HA	2.13	0.47
3:D:158:LEU:HA	3:D:158:LEU:HD12	1.64	0.47
1:A:919:TYR:HB3	1:A:921:PHE:HE2	1.79	0.47
2:B:255:LEU:HD11	2:B:1059:LEU:HD23	1.96	0.47
2:C:1072:ASN:HB3	2:C:1172:GLU:HG2	1.95	0.47
3:E:44:LEU:HD11	3:E:256:GLY:HA3	1.95	0.47
2:B:1330:ILE:HA	2:B:1330:ILE:HD13	1.68	0.47
2:B:617:ASP:OD1	2:B:618:LEU:N	2.47	0.47
2:C:164:LEU:HD23	2:C:208:LEU:HA	1.96	0.47
1:A:251:VAL:HG12	1:A:253:ALA:H	1.80	0.47
2:B:512:LEU:HD21	2:B:687:LEU:HD12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:873:TYR:HA	2:B:896:LEU:O	2.14	0.47
3:D:148:ASP:OD1	3:D:151:ASP:N	2.39	0.47
3:D:185:SER:O	3:D:189:LEU:HB2	2.15	0.47
1:A:726:ILE:HD12	1:A:743:PRO:HG3	1.97	0.47
2:B:489:MET:SD	2:B:527:ARG:HD2	2.55	0.47
2:C:517:PHE:CD1	2:C:760:THR:HG22	2.49	0.47
1:A:904:PHE:H	4:A:1101:SAM:C2	2.27	0.47
2:B:338:ARG:HB3	2:B:340:VAL:HG13	1.97	0.47
2:C:828:ASP:OD2	2:C:960:THR:OG1	2.30	0.47
2:B:164:LEU:HD21	2:B:1067:ILE:HD11	1.96	0.47
3:D:213:LEU:HD11	3:D:217:LYS:HE3	1.97	0.47
3:D:273:LEU:O	3:D:277:GLU:HG3	2.14	0.47
3:E:56:LEU:HD23	3:E:136:LYS:HG3	1.96	0.47
1:A:106:SER:OG	1:A:108:ASP:OD1	2.20	0.46
2:B:482:ILE:HG23	2:B:706:TYR:OH	2.15	0.46
2:C:254:VAL:HB	2:C:1062:ILE:HD11	1.97	0.46
2:C:144:ASN:HD21	2:C:391:GLY:HA2	1.80	0.46
2:B:1278:TYR:CE1	2:B:1290:LYS:HA	2.50	0.46
2:B:540:PHE:CE2	2:B:600:ILE:HG23	2.50	0.46
3:D:253:GLU:HA	3:D:254:TYR:HA	1.46	0.46
3:E:96:LEU:HA	3:E:101:THR:HG21	1.98	0.46
1:A:895:LYS:HB2	1:A:897:ILE:HG12	1.96	0.46
2:B:1022:ILE:HG22	2:B:1028:VAL:HG22	1.96	0.46
3:D:28:PRO:CB	3:D:226:MET:HG3	2.45	0.46
2:B:949:ALA:HB1	2:B:960:THR:HG22	1.98	0.46
2:C:883:ILE:HD13	2:C:910:LEU:HD21	1.97	0.46
3:D:182:TRP:NE1	3:D:185:SER:HA	2.30	0.46
1:A:746:PHE:HB2	1:A:785:ALA:HB3	1.97	0.46
1:A:943:ILE:HA	1:A:946:VAL:HG12	1.96	0.46
2:B:1077:MET:HG2	2:B:1079:LEU:HD13	1.97	0.46
2:B:347:ALA:HA	2:B:1301:VAL:HA	1.97	0.46
2:B:495:LEU:HD22	2:B:532:ILE:HG13	1.96	0.46
1:A:401:ILE:HD12	1:A:747:CYS:SG	2.56	0.46
1:A:28:PRO:HA	1:A:97:ARG:HG2	1.96	0.46
2:B:228:VAL:HG11	2:B:231:LEU:HD12	1.98	0.46
2:C:1243:ARG:HB3	2:C:1258:VAL:HG23	1.98	0.46
3:D:45:VAL:HG22	3:D:171:VAL:HG12	1.98	0.46
3:D:258:ASN:ND2	3:D:260:MET:SD	2.88	0.46
1:A:403:ILE:HG22	1:A:827:ARG:HG3	1.98	0.46
2:B:454:GLU:OE2	2:B:467:LYS:NZ	2.41	0.46
1:A:218:THR:OG1	1:A:220:HIS:NE2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:LEU:HA	1:A:337:LEU:HD13	1.80	0.46
1:A:947:ALA:HB1	1:A:1012:ILE:HG21	1.97	0.46
2:B:357:VAL:HG13	2:B:1054:ARG:HD3	1.98	0.46
2:B:529:LYS:HD2	2:B:589:PHE:CD2	2.51	0.46
2:C:186:ASP:CG	2:C:279:SER:H	2.19	0.46
2:C:588:LEU:HA	2:C:588:LEU:HD23	1.81	0.46
3:D:56:LEU:HD23	3:D:56:LEU:HA	1.76	0.46
1:A:398:GLU:HG3	1:A:402:THR:HB	1.97	0.46
2:B:1209:GLY:O	2:B:1212:ARG:HG2	2.16	0.46
2:C:1101:TYR:HB2	2:C:1141:ILE:HG12	1.98	0.46
2:C:1271:SER:N	2:C:1275:ASP:O	2.44	0.46
2:C:171:GLU:HB2	2:C:1211:LEU:HD13	1.97	0.46
3:D:78:GLY:O	3:D:275:ARG:NH2	2.44	0.46
3:E:193:VAL:HG21	3:E:230:ILE:HG13	1.98	0.46
2:B:842:ASP:HB2	2:B:845:GLU:HG3	1.98	0.46
2:B:953:ASP:OD1	2:B:960:THR:OG1	2.27	0.46
2:C:409:ILE:O	2:C:413:MET:HG2	2.16	0.46
3:D:232:SER:HA	3:D:235:VAL:HG22	1.97	0.45
3:D:77:PHE:HB3	3:D:230:ILE:HG21	1.98	0.45
3:E:148:ASP:OD2	3:E:151:ASP:N	2.39	0.45
3:E:262:THR:HG22	3:E:272:ASP:HA	1.98	0.45
1:A:1034:ARG:HH21	1:A:1036:GLY:HA2	1.80	0.45
2:B:1243:ARG:HD3	2:B:1256:GLY:O	2.15	0.45
2:B:738:GLU:OE1	2:B:858:HIS:HD2	1.98	0.45
2:B:959:GLN:HG3	2:B:964:VAL:HG21	1.98	0.45
2:C:822:MET:O	2:C:825:SER:OG	2.33	0.45
2:C:98:ASN:ND2	2:C:101:ASP:OD1	2.49	0.45
1:A:864:ARG:HB3	1:A:864:ARG:HE	1.56	0.45
2:C:1051:GLN:O	2:C:1055:LEU:HB2	2.15	0.45
1:A:79:PRO:HA	1:A:80:SER:HA	1.58	0.45
2:B:1075:ARG:NH2	2:B:1167:ASP:OD1	2.45	0.45
2:B:226:PRO:HB2	2:B:250:GLY:HA3	1.99	0.45
2:C:1201:LEU:HD12	2:C:1201:LEU:HA	1.73	0.45
2:B:891:HIS:CD2	3:D:240:VAL:HG21	2.52	0.45
1:A:613:ILE:HD11	1:A:642:ALA:HB3	1.98	0.45
2:B:1148:SER:HB3	2:B:1151:VAL:HG23	1.97	0.45
2:B:759:ASP:OD2	2:B:761:SER:OG	2.35	0.45
1:A:734:ILE:HG12	1:A:746:PHE:CE1	2.52	0.45
2:C:204:VAL:HB	2:C:1242:MET:HB2	1.99	0.45
2:C:700:ASP:HB3	2:C:1326:ARG:HG2	1.97	0.45
2:C:190:VAL:HG23	2:C:300:LEU:HD22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:529:LYS:HD2	2:C:589:PHE:CD2	2.52	0.45
2:C:609:PRO:HB2	2:C:634:TYR:CE2	2.51	0.45
3:E:160:LEU:HD11	3:E:229:PHE:HA	1.98	0.45
1:A:1056:VAL:O	1:A:1057:ARG:HD2	2.17	0.45
1:A:199:MET:HG3	1:A:205:VAL:HG21	1.99	0.45
1:A:278:LEU:HA	1:A:278:LEU:HD23	1.68	0.45
3:E:229:PHE:O	3:E:233:THR:HG23	2.17	0.45
1:A:238:ASP:OD2	1:A:259:ARG:NE	2.36	0.45
1:A:741:TYR:CZ	1:A:746:PHE:HZ	2.35	0.45
1:A:7:ILE:HG13	1:A:250:LEU:HD11	1.98	0.45
2:C:307:VAL:HA	2:C:1247:ASN:ND2	2.32	0.45
2:C:833:ARG:HD2	2:C:941:TYR:CD2	2.52	0.45
1:A:473:VAL:HG11	1:A:494:THR:HG23	1.98	0.45
1:A:677:LEU:HG	1:A:706:TYR:CE2	2.52	0.45
1:A:772:TRP:HH2	1:A:784:ILE:HD11	1.82	0.45
2:C:626:ARG:HG2	2:C:631:PRO:HB3	1.99	0.45
3:E:19:ILE:HD11	3:E:31:PHE:HB2	1.99	0.45
1:A:1006:MET:HA	1:A:1009:ASP:OD2	2.17	0.45
1:A:890:LEU:HD13	1:A:891:THR:N	2.32	0.45
2:B:547:GLU:HG2	2:B:599:THR:OG1	2.17	0.45
2:B:616:ASP:O	2:B:620:ILE:HG13	2.16	0.45
2:B:543:TRP:CH2	2:B:666:ARG:HG2	2.52	0.45
2:B:891:HIS:CG	3:D:240:VAL:HG21	2.52	0.45
3:E:159:GLU:O	3:E:225:ARG:HG2	2.17	0.45
1:A:42:PHE:CZ	1:A:44:SER:HA	2.51	0.44
1:A:93:HIS:NE2	1:A:97:ARG:HD2	2.33	0.44
2:B:1139:MET:HB3	2:B:1166:VAL:HG12	1.99	0.44
2:B:1214:GLU:HG2	2:B:1215:PRO:HD2	1.98	0.44
2:B:1233:LEU:HD13	2:B:1233:LEU:HA	1.66	0.44
2:B:332:THR:HA	2:B:344:VAL:HG12	1.99	0.44
1:A:114:ASN:HD22	1:A:149:ALA:HB1	1.81	0.44
1:A:869:ILE:O	1:A:872:VAL:HG12	2.17	0.44
2:B:169:LYS:O	2:B:202:ALA:N	2.46	0.44
2:B:447:ARG:HH22	2:B:770:CYS:N	2.15	0.44
2:C:1076:ILE:HB	2:C:1166:VAL:HG22	2.00	0.44
2:C:1212:ARG:HA	2:C:1213:PRO:HD2	1.82	0.44
2:C:289:THR:O	2:C:328:GLY:HA3	2.16	0.44
2:C:515:ILE:HD12	2:C:659:LEU:HD11	1.99	0.44
2:B:774:LEU:HA	2:B:774:LEU:HD23	1.78	0.44
2:C:1031:TYR:HH	2:C:1038:GLU:HA	1.81	0.44
3:E:93:LEU:HD23	3:E:93:LEU:HA	1.63	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:495:LEU:HB2	2:B:528:ILE:HD12	1.98	0.44
2:B:921:ASP:O	2:B:928:ARG:NH1	2.51	0.44
2:C:171:GLU:OE2	2:C:1181:SER:OG	2.34	0.44
2:C:615:THR:H	2:C:1333:ALA:HA	1.82	0.44
2:C:646:ASN:HD21	2:C:699:THR:HG21	1.81	0.44
1:A:256:VAL:HG22	1:A:335:LEU:HD13	2.00	0.44
1:A:679:LYS:HE3	1:A:714:ARG:HH21	1.81	0.44
2:B:704:VAL:HG12	2:B:1330:ILE:HD11	2.00	0.44
2:C:196:LEU:HD12	2:C:196:LEU:HA	1.87	0.44
2:C:227:LEU:HD22	2:C:246:GLU:HB2	1.99	0.44
2:C:775:VAL:HA	2:C:776:ARG:HA	1.62	0.44
2:C:850:THR:HG22	2:C:916:LEU:HD11	1.99	0.44
3:D:68:ILE:HA	3:D:68:ILE:HD12	1.74	0.44
2:B:362:LEU:HD22	2:B:1303:SER:OG	2.18	0.44
2:B:176:LYS:HE2	2:B:176:LYS:HB2	1.60	0.44
2:C:699:THR:OG1	2:C:700:ASP:OD2	2.33	0.44
3:D:102:SER:O	3:D:114:SER:HA	2.18	0.44
1:A:278:LEU:HD21	1:A:315:LEU:HD11	2.00	0.44
1:A:849:ILE:HD12	1:A:871:VAL:HG12	2.00	0.44
2:B:1305:MET:HE2	2:B:1309:ILE:HG21	2.00	0.44
2:B:267:VAL:HG13	2:B:291:HIS:HE1	1.82	0.44
2:B:846:GLY:O	2:B:911:ARG:HG3	2.17	0.44
2:B:843:LEU:HG	2:B:942:HIS:CG	2.52	0.44
2:C:303:ASP:N	2:C:311:ASN:OD1	2.48	0.44
2:C:674:LYS:HA	2:C:674:LYS:HD2	1.64	0.44
2:C:736:SER:HB3	2:C:1017:ALA:HA	2.00	0.44
1:A:308:ALA:HB1	1:A:312:LEU:HB3	1.99	0.44
2:C:94:PHE:HB3	2:C:105:MET:HG2	1.99	0.44
2:C:150:LEU:HD21	2:C:399:PRO:HD2	2.00	0.44
2:C:633:THR:HG21	2:C:710:SER:HB2	1.99	0.44
3:D:239:VAL:CG1	3:D:250:ARG:HD2	2.47	0.44
1:A:282:GLU:OE1	1:A:810:ARG:NH2	2.51	0.44
1:A:936:ALA:HA	1:A:939:GLN:HG3	1.99	0.44
2:B:762:ILE:HA	2:B:762:ILE:HD12	1.88	0.44
2:B:1170:ASP:OD1	2:B:1198:LYS:HE2	2.18	0.43
2:C:163:TYR:O	2:C:209:ASN:N	2.40	0.43
2:C:446:LYS:HB3	2:C:448:TYR:CD2	2.52	0.43
2:C:873:TYR:HA	2:C:896:LEU:O	2.18	0.43
3:D:19:ILE:H	3:D:19:ILE:HG13	1.73	0.43
1:A:388:VAL:HG23	1:A:736:GLY:HA3	2.01	0.43
2:B:629:ARG:HH11	2:B:1037:ILE:HA	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:204:VAL:HG12	2:B:1241:SER:HB3	1.99	0.43
2:B:478:ILE:HG23	2:B:766:ILE:HD11	2.00	0.43
1:A:114:ASN:OD1	1:A:117:LEU:HB2	2.18	0.43
1:A:143:TYR:CG	1:A:149:ALA:HB2	2.53	0.43
1:A:812:VAL:HA	1:A:813:PRO:HA	1.79	0.43
2:B:223:LYS:HB3	2:B:1174:THR:HG21	2.00	0.43
2:C:478:ILE:HG12	2:C:762:ILE:HD11	2.01	0.43
2:C:816:PRO:HB3	2:C:986:ILE:HG22	2.00	0.43
2:B:1270:LEU:HA	2:B:1270:LEU:HD23	1.66	0.43
2:B:462:LEU:HD12	2:B:506:SER:HB3	1.99	0.43
2:C:600:ILE:O	2:C:604:MET:HG2	2.18	0.43
2:B:147:VAL:HG22	2:B:379:LEU:HD11	2.00	0.43
2:B:385:ILE:H	2:B:385:ILE:HG12	1.59	0.43
2:B:405:HIS:ND1	2:B:625:PRO:HA	2.34	0.43
2:B:765:PRO:HA	2:B:769:GLN:HG2	2.01	0.43
2:B:947:GLU:OE1	2:B:968:ARG:NH2	2.46	0.43
2:C:1075:ARG:NH1	2:C:1090:PRO:O	2.52	0.43
2:C:931:ASN:HD21	2:C:936:MET:HB3	1.84	0.43
3:E:53:GLU:CD	3:E:53:GLU:H	2.21	0.43
1:A:62:PHE:HB2	1:A:67:ARG:HD3	1.99	0.43
1:A:828:TYR:HA	1:A:1032:GLY:O	2.18	0.43
2:B:707:ALA:O	2:B:710:SER:HB3	2.19	0.43
2:C:714:LEU:HD23	2:C:714:LEU:HA	1.87	0.43
1:A:864:ARG:HD3	4:A:1101:SAM:HG2	2.01	0.43
2:B:1159:VAL:HA	2:B:1164:TRP:HB2	2.01	0.43
2:C:156:GLN:NE2	2:C:1308:ASN:OD1	2.52	0.43
2:C:352:HIS:O	2:C:356:SER:OG	2.22	0.43
3:D:229:PHE:O	3:D:233:THR:HG23	2.19	0.43
3:E:70:ASP:O	3:E:74:GLN:HB2	2.19	0.43
2:B:557:THR:OG1	2:B:558:TYR:N	2.50	0.43
2:C:325:TYR:HA	2:C:1267:THR:CG2	2.48	0.43
2:C:154:PHE:CE2	2:C:365:LEU:HB2	2.54	0.43
2:C:862:ARG:NH1	2:C:948:ILE:HG12	2.34	0.43
3:D:4:GLN:HA	3:D:5:PRO:HD3	1.90	0.43
1:A:462:ILE:HG12	1:A:682:SER:O	2.19	0.43
2:B:948:ILE:HA	2:B:948:ILE:HD12	1.74	0.43
2:C:528:ILE:HA	2:C:577:GLN:NE2	2.33	0.43
3:E:137:LEU:HD21	3:E:282:PHE:HB2	2.01	0.43
1:A:184:TRP:HB3	1:A:195:ILE:HD13	2.00	0.43
1:A:207:THR:CG2	1:A:218:THR:HG22	2.48	0.43
1:A:886:ARG:H	1:A:886:ARG:HG3	1.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:515:ILE:H	2:B:515:ILE:HG12	1.53	0.43
2:B:546:VAL:O	2:B:550:ILE:HG13	2.19	0.43
2:C:1050:LEU:HD12	2:C:1050:LEU:HA	1.84	0.43
2:C:1097:VAL:HG11	2:C:1123:PRO:HG2	2.00	0.43
2:B:419:TYR:CG	2:B:1005:LEU:HD13	2.54	0.42
2:C:1175:ALA:HA	2:C:1204:LEU:O	2.19	0.42
2:C:152:ASP:N	2:C:152:ASP:OD1	2.46	0.42
1:A:204:LEU:HB3	1:A:221:TYR:HB2	2.01	0.42
2:B:414:LEU:HD12	2:B:414:LEU:HA	1.70	0.42
2:B:511:VAL:O	2:B:515:ILE:HG12	2.19	0.42
2:C:251:LEU:HA	2:C:251:LEU:HD23	1.76	0.42
1:A:537:VAL:HG13	1:A:550:TYR:CE2	2.53	0.42
2:B:1033:ASP:O	2:B:1034:GLN:HB2	2.19	0.42
2:C:157:ILE:HG12	2:C:263:ARG:HB3	2.00	0.42
1:A:841:MET:HA	1:A:1019:PRO:HG3	2.02	0.42
1:A:565:ARG:HA	1:A:565:ARG:HD3	1.74	0.42
2:B:886:SER:O	2:B:890:THR:HG23	2.20	0.42
2:C:1022:ILE:HG22	2:C:1028:VAL:HA	2.01	0.42
2:C:502:PHE:O	2:C:542:ARG:HG2	2.19	0.42
2:C:890:THR:OG1	2:C:892:VAL:HG12	2.19	0.42
3:D:7:GLY:HA3	3:D:11:THR:HG21	2.01	0.42
3:D:133:THR:OG1	3:D:134:TYR:N	2.51	0.42
1:A:179:TYR:HB3	1:A:221:TYR:CD1	2.54	0.42
1:A:456:PHE:HD1	1:A:456:PHE:HA	1.67	0.42
2:C:637:TYR:OH	2:C:702:LEU:HD23	2.19	0.42
3:D:187:ILE:HD13	3:D:187:ILE:HA	1.92	0.42
1:A:681:ALA:HA	1:A:1041:ALA:HB2	2.00	0.42
1:A:977:HIS:O	1:A:981:ARG:HB3	2.19	0.42
2:B:1289:PRO:HD2	3:D:20:ARG:HD2	2.01	0.42
2:B:255:LEU:HD23	2:B:819:PHE:CZ	2.54	0.42
3:E:105:LEU:HD13	3:E:111:ILE:HG12	2.02	0.42
3:E:240:VAL:O	3:E:250:ARG:HD3	2.20	0.42
2:B:147:VAL:HG11	2:B:375:ARG:HB3	2.02	0.42
2:B:537:LEU:HA	2:B:537:LEU:HD23	1.73	0.42
2:B:793:TYR:HA	2:B:794:PRO:HD3	1.88	0.42
2:B:931:ASN:OD1	2:B:931:ASN:N	2.40	0.42
3:D:69:GLU:O	3:D:73:THR:OG1	2.30	0.42
1:A:453:LEU:HA	1:A:1025:ILE:HD11	2.02	0.42
1:A:324:ARG:O	1:A:349:TYR:OH	2.28	0.42
1:A:398:GLU:HA	1:A:401:ILE:O	2.19	0.42
1:A:406:VAL:HG13	1:A:1034:ARG:HD2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:644:THR:O	1:A:696:PRO:HD2	2.19	0.42
2:B:924:ASP:O	2:B:927:SER:OG	2.29	0.42
2:C:348:LEU:HD12	2:C:1302:VAL:HG21	2.00	0.42
2:C:664:ASN:HB2	2:C:681:LYS:NZ	2.34	0.42
1:A:417:TYR:CD1	1:A:537:VAL:HG21	2.55	0.42
2:B:379:LEU:HD23	2:B:379:LEU:HA	1.89	0.42
2:B:659:LEU:HD23	2:B:659:LEU:HA	1.84	0.42
2:C:168:VAL:HG11	2:C:196:LEU:HG	2.02	0.42
3:D:188:SER:O	3:D:191:ARG:HG3	2.19	0.42
3:D:35:LEU:HD12	3:D:35:LEU:HA	1.79	0.42
2:B:336:TYR:HD2	3:D:89:TYR:CE2	2.37	0.42
1:A:1007:LEU:HA	1:A:1007:LEU:HD12	1.79	0.42
1:A:114:ASN:HA	1:A:143:TYR:HE2	1.85	0.42
1:A:894:LYS:HD3	1:A:894:LYS:HA	1.73	0.42
2:B:1193:ILE:HA	2:B:1193:ILE:HD13	1.74	0.42
2:B:685:ARG:O	2:B:689:THR:HG23	2.19	0.42
1:A:183:ILE:HG12	1:A:183:ILE:H	1.56	0.41
1:A:36:THR:O	1:A:54:LEU:HB2	2.20	0.41
1:A:415:ASP:HB3	1:A:1038:THR:HG21	2.01	0.41
1:A:728:PRO:HG3	1:A:828:TYR:CE2	2.54	0.41
2:B:806:VAL:O	2:B:810:LEU:HG	2.20	0.41
2:B:885:ALA:HA	2:B:888:GLN:HE21	1.85	0.41
2:C:1211:LEU:HA	2:C:1211:LEU:HD23	1.68	0.41
2:C:307:VAL:HA	2:C:1247:ASN:HD21	1.85	0.41
2:C:450:PRO:HG3	2:C:686:HIS:CB	2.49	0.41
2:C:537:LEU:HA	2:C:537:LEU:HD23	1.74	0.41
2:C:852:TYR:CZ	2:C:856:LEU:HD21	2.54	0.41
3:E:153:TYR:O	3:E:156:VAL:HB	2.20	0.41
1:A:714:ARG:NE	1:A:1044:ASP:OD2	2.53	0.41
1:A:765:TYR:HA	1:A:792:ILE:HG13	2.01	0.41
2:B:1176:GLU:HB2	2:B:1203:HIS:CE1	2.55	0.41
2:C:1193:ILE:HD12	2:C:1202:PHE:CE1	2.55	0.41
2:C:636:PRO:HG2	2:C:706:TYR:CE2	2.54	0.41
1:A:561:LEU:HD23	1:A:561:LEU:N	2.36	0.41
1:A:788:ASP:HA	1:A:789:PRO:HD3	1.88	0.41
2:B:392:PRO:HD2	2:B:1315:MET:HE2	2.02	0.41
2:B:425:ILE:HG13	2:B:1004:PHE:HD2	1.85	0.41
2:C:1025:ASP:OD1	2:C:1027:THR:HG23	2.20	0.41
2:C:1230:ILE:H	2:C:1230:ILE:HG12	1.74	0.41
3:D:123:ASP:O	3:D:127:VAL:HG23	2.20	0.41
3:E:253:GLU:HA	3:E:254:TYR:HA	1.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:PHE:HE1	1:A:47:ARG:HA	1.84	0.41
2:C:1116:ARG:HH11	2:C:1116:ARG:HB3	1.84	0.41
2:C:414:LEU:HD12	2:C:414:LEU:HA	1.92	0.41
2:C:750:GLU:OE1	2:C:1003:ARG:NH1	2.44	0.41
2:C:838:GLU:HB2	2:C:911:ARG:HH21	1.84	0.41
1:A:528:SER:O	1:A:532:MET:HG2	2.20	0.41
1:A:710:ALA:HB2	1:A:1048:HIS:HB3	2.02	0.41
2:B:1278:TYR:CD2	2:B:1290:LYS:HE2	2.56	0.41
2:B:278:LEU:HD22	2:B:282:VAL:HG11	2.03	0.41
2:B:482:ILE:HG23	2:B:706:TYR:CZ	2.55	0.41
2:B:529:LYS:HB2	2:B:589:PHE:CE2	2.56	0.41
2:C:1049:GLU:O	2:C:1053:ARG:HG2	2.20	0.41
1:A:828:TYR:O	1:A:1034:ARG:HG2	2.21	0.41
2:B:810:LEU:HA	2:B:810:LEU:HD23	1.83	0.41
2:C:1267:THR:HB	2:C:1299:SER:CB	2.50	0.41
2:B:769:GLN:HB2	2:B:769:GLN:HE21	1.74	0.41
2:C:1233:LEU:HA	2:C:1233:LEU:HD12	1.67	0.41
3:E:156:VAL:HG22	3:E:228:LEU:HD22	2.02	0.41
1:A:764:SER:HB2	1:A:765:TYR:CE2	2.55	0.41
2:B:227:LEU:HA	2:B:246:GLU:O	2.21	0.41
2:B:271:THR:O	2:B:289:THR:HA	2.21	0.41
2:B:343:ILE:HD12	2:B:362:LEU:HD11	2.02	0.41
2:B:382:HIS:HA	2:B:712:PHE:CE1	2.56	0.41
2:B:639:ASN:OD1	2:B:639:ASN:N	2.54	0.41
2:B:659:LEU:O	2:B:663:VAL:HG23	2.21	0.41
2:B:714:LEU:HD23	2:B:714:LEU:HA	1.61	0.41
2:C:251:LEU:HD22	2:C:1062:ILE:HG13	2.02	0.41
2:C:223:LYS:HZ2	2:C:1203:HIS:HB2	1.86	0.41
2:C:1060:ARG:HD3	2:C:1291:LEU:O	2.20	0.41
3:E:35:LEU:HD21	3:E:229:PHE:CE2	2.55	0.41
4:A:1101:SAM:HB2	4:A:1101:SAM:HE1	1.85	0.41
1:A:46:ARG:N	1:A:46:ARG:HD2	2.36	0.41
2:B:1220:PRO:HA	2:B:1221:PRO:HD3	1.90	0.41
2:B:347:ALA:HB1	2:B:1267:THR:OG1	2.21	0.41
2:B:135:LYS:HB3	2:B:136:VAL:H	1.67	0.41
2:B:492:VAL:HB	2:B:747:ARG:HG2	2.03	0.41
2:C:1023:ARG:HG2	2:C:1024:PRO:HD2	2.02	0.41
2:C:102:VAL:HG23	2:C:102:VAL:H	1.66	0.41
2:C:1064:ASN:HA	2:C:1065:PRO:HD3	1.91	0.41
3:D:28:PRO:HG3	3:D:223:VAL:HG22	2.02	0.41
2:C:366:MET:HG2	3:E:266:THR:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:TYR:HB2	1:A:678:LEU:HG	2.03	0.41
1:A:773:ARG:O	1:A:818:PHE:HA	2.21	0.41
1:A:912:ASP:OD1	1:A:912:ASP:N	2.52	0.41
2:B:243:GLN:O	2:B:246:GLU:HB2	2.20	0.41
2:B:709:MET:HG2	2:B:712:PHE:CE2	2.56	0.41
2:B:728:LYS:HA	2:B:728:LYS:HD3	1.84	0.41
2:B:798:THR:O	2:B:802:GLN:HG2	2.21	0.41
2:C:1092:VAL:HA	2:C:1093:PRO:HD3	1.92	0.41
2:C:244:SER:HB2	2:C:1201:LEU:HD13	2.03	0.41
3:E:19:ILE:HG23	3:E:196:TRP:CZ2	2.56	0.41
1:A:289:ASP:OD1	1:A:291:SER:OG	2.37	0.41
1:A:658:ILE:O	1:A:662:ILE:HG12	2.20	0.41
2:B:338:ARG:HD2	2:B:338:ARG:N	2.35	0.41
2:B:514:PHE:CD2	2:B:532:ILE:HG23	2.56	0.41
2:B:809:VAL:O	2:B:813:LEU:HB2	2.21	0.41
2:B:820:ILE:HD13	2:B:820:ILE:HA	1.92	0.41
2:B:835:TYR:CD2	2:B:941:TYR:HB3	2.56	0.41
2:B:836:GLN:OE1	2:B:836:GLN:N	2.55	0.41
2:C:1267:THR:HB	2:C:1299:SER:HB3	2.03	0.41
2:C:375:ARG:HE	2:C:375:ARG:HB2	1.60	0.41
3:E:185:SER:O	3:E:189:LEU:HB2	2.21	0.41
2:B:1219:ASP:HA	2:B:1220:PRO:HD3	1.83	0.40
2:B:875:THR:HG23	2:B:877:ALA:H	1.86	0.40
2:C:1080:THR:HG22	2:C:1227:MET:SD	2.61	0.40
2:C:244:SER:HB3	2:C:1199:GLY:O	2.20	0.40
2:C:171:GLU:HG3	2:C:1211:LEU:HB3	2.02	0.40
2:C:213:PHE:CE1	2:C:254:VAL:HG13	2.56	0.40
2:C:419:TYR:HA	2:C:420:PRO:HD2	1.91	0.40
3:E:44:LEU:HD13	3:E:154:ALA:HA	2.03	0.40
1:A:967:ILE:HD12	1:A:987:LEU:HD12	2.03	0.40
2:B:354:ALA:O	2:B:358:LEU:HG	2.21	0.40
2:B:541:SER:HA	2:B:548:TYR:CG	2.56	0.40
3:D:14:GLN:HE22	3:D:107:LEU:HD23	1.87	0.40
3:E:123:ASP:HA	3:E:124:PRO:HD3	1.88	0.40
1:A:166:ILE:HD11	1:A:178:PRO:HD2	2.04	0.40
1:A:427:ASP:HB3	1:A:703:PHE:CD1	2.57	0.40
2:B:330:THR:HG23	2:B:331:GLU:H	1.86	0.40
2:C:1013:LYS:HE2	2:C:1015:GLN:HE21	1.85	0.40
2:C:301:LEU:HB3	2:C:305:THR:HG22	2.04	0.40
2:C:248:VAL:HG13	2:C:970:LEU:HB3	2.03	0.40
3:D:75:ALA:O	3:D:275:ARG:HD2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:ALA:HB1	1:A:187:PRO:HA	2.02	0.40
1:A:460:VAL:HG12	1:A:465:LEU:HD11	2.03	0.40
1:A:928:GLU:HG2	1:A:934:THR:HG22	2.04	0.40
2:B:267:VAL:HG22	2:B:1304:MET:HG3	2.03	0.40
2:B:193:THR:HA	2:B:296:VAL:HG12	2.04	0.40
2:B:489:MET:HE3	2:B:580:TYR:HE2	1.86	0.40
2:C:603:ILE:HD11	2:C:662:VAL:HG21	2.03	0.40
1:A:161:TYR:HB2	1:A:183:ILE:O	2.22	0.40
1:A:236:LEU:HD21	1:A:240:ARG:HH21	1.87	0.40
1:A:711:MET:HG2	1:A:711:MET:H	1.69	0.40
1:A:40:TYR:OH	1:A:83:ILE:HG13	2.22	0.40
1:A:797:ARG:HD2	1:A:869:ILE:HD11	2.03	0.40
2:B:493:HIS:O	2:B:577:GLN:NE2	2.54	0.40
2:B:926:VAL:HG22	2:B:936:MET:HG2	2.03	0.40
2:C:253:MET:N	2:C:253:MET:SD	2.93	0.40
2:C:650:SER:HA	2:C:653:ARG:CZ	2.52	0.40
2:C:795:ASP:O	2:C:798:THR:HG22	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1055/1058 (100%)	1004 (95%)	45 (4%)	6 (1%)	30	68
2	B	1187/1333 (89%)	1135 (96%)	49 (4%)	3 (0%)	46	80
2	C	1246/1333 (94%)	1181 (95%)	60 (5%)	5 (0%)	39	75
3	D	290/448 (65%)	281 (97%)	8 (3%)	1 (0%)	46	80
3	E	290/448 (65%)	281 (97%)	9 (3%)	0	100	100
All	All	4068/4620 (88%)	3882 (95%)	171 (4%)	15 (0%)	43	75

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	186	ALA
2	C	1145	ALA
2	C	1251	VAL
2	B	1123	PRO
3	D	244	VAL
1	A	483	MET
1	A	979	THR
2	C	1267	THR
1	A	728	PRO
2	B	288	THR
2	B	1068	ALA
1	A	854	ASN
1	A	884	ALA
2	C	775	VAL
2	C	1093	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	942/943 (100%)	829 (88%)	113 (12%)	6	24
2	B	1038/1153 (90%)	963 (93%)	75 (7%)	18	53
2	C	1089/1153 (94%)	980 (90%)	109 (10%)	9	34
3	D	240/379 (63%)	215 (90%)	25 (10%)	9	32
3	E	240/379 (63%)	222 (92%)	18 (8%)	17	51
All	All	3549/4007 (89%)	3209 (90%)	340 (10%)	15	37

All (340) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	THR
1	A	39	LEU
1	A	46	ARG

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Mol	Chain	Res	Type
1	A	47	ARG
1	A	52	ARG
1	A	74	LEU
1	A	76	LEU
1	A	83	ILE
1	A	88	LEU
1	A	92	LEU
1	A	110	THR
1	A	117	LEU
1	A	128	THR
1	A	133	LEU
1	A	157	LEU
1	A	166	ILE
1	A	185	HIS
1	A	199	MET
1	A	205	VAL
1	A	222	ARG
1	A	234	LYS
1	A	254	ASP
1	A	260	LEU
1	A	272	LEU
1	A	275	ILE
1	A	284	THR
1	A	293	LEU
1	A	300	LEU
1	A	311	GLN
1	A	312	LEU
1	A	315	LEU
1	A	324	ARG
1	A	335	LEU
1	A	337	LEU
1	A	340	ILE
1	A	346	ILE
1	A	357	THR
1	A	358	ILE
1	A	362	MET
1	A	379	VAL
1	A	388	VAL
1	A	390	ASP
1	A	401	ILE
1	A	402	THR
1	A	405	MET

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Mol	Chain	Res	Type
1	A	420	VAL
1	A	421	LEU
1	A	429	TRP
1	A	444	LEU
1	A	456	PHE
1	A	464	ASP
1	A	466	LEU
1	A	483	MET
1	A	486	THR
1	A	494	THR
1	A	503	ILE
1	A	504	THR
1	A	518	TYR
1	A	523	MET
1	A	545	PHE
1	A	551	LEU
1	A	561	LEU
1	A	583	ARG
1	A	587	MET
1	A	626	GLU
1	A	628	MET
1	A	647	LEU
1	A	648	VAL
1	A	668	LEU
1	A	680	THR
1	A	692	ILE
1	A	719	VAL
1	A	723	GLU
1	A	724	MET
1	A	726	ILE
1	A	731	HIS
1	A	738	SER
1	A	746	PHE
1	A	747	CYS
1	A	763	LYS
1	A	765	TYR
1	A	780	LEU
1	A	782	ASN
1	A	792	ILE
1	A	824	ARG
1	A	832	GLU
1	A	833	VAL

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Mol	Chain	Res	Type
1	A	849	ILE
1	A	866	LEU
1	A	877	LYS
1	A	886	ARG
1	A	890	LEU
1	A	902	ARG
1	A	910	ASN
1	A	918	ILE
1	A	925	ILE
1	A	926	MET
1	A	941	ASP
1	A	951	LEU
1	A	952	THR
1	A	960	ILE
1	A	967	ILE
1	A	970	ARG
1	A	971	LEU
1	A	981	ARG
1	A	996	ASP
1	A	1007	LEU
1	A	1013	THR
1	A	1018	ARG
1	A	1024	LEU
1	A	1025	ILE
1	A	1034	ARG
1	A	1035	LEU
2	B	144	ASN
2	B	147	VAL
2	B	165	THR
2	B	176	LYS
2	B	190	VAL
2	B	217	THR
2	B	223	LYS
2	B	233	VAL
2	B	235	ILE
2	B	264	LEU
2	B	280	THR
2	B	291	HIS
2	B	293	ASN
2	B	294	VAL
2	B	315	THR
2	B	323	THR

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Mol	Chain	Res	Type
2	B	329	LEU
2	B	330	THR
2	B	335	ASP
2	B	340	VAL
2	B	384	MET
2	B	477	SER
2	B	506	SER
2	B	510	VAL
2	B	515	ILE
2	B	533	GLN
2	B	557	THR
2	B	605	ARG
2	B	633	THR
2	B	637	TYR
2	B	640	GLN
2	B	647	GLU
2	B	661	ASN
2	B	689	THR
2	B	708	THR
2	B	740	SER
2	B	748	GLN
2	B	755	LEU
2	B	767	LEU
2	B	774	LEU
2	B	797	SER
2	B	799	THR
2	B	802	GLN
2	B	811	SER
2	B	815	LEU
2	B	851	THR
2	B	912	GLU
2	B	921	ASP
2	B	931	ASN
2	B	946	LEU
2	B	948	ILE
2	B	966	GLN
2	B	976	THR
2	B	1036	ASP
2	B	1050	LEU
2	B	1052	LEU
2	B	1060	ARG
2	B	1061	LEU

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Mol	Chain	Res	Type
2	B	1062	ILE
2	B	1092	VAL
2	B	1110	LEU
2	B	1120	THR
2	B	1132	THR
2	B	1179	THR
2	B	1193	ILE
2	B	1228	ARG
2	B	1233	LEU
2	B	1234	GLN
2	B	1249	ASN
2	B	1262	SER
2	B	1269	THR
2	B	1270	LEU
2	B	1294	ASP
2	B	1311	THR
2	B	1331	ARG
2	C	74	LYS
2	C	77	THR
2	C	98	ASN
2	C	116	SER
2	C	118	THR
2	C	120	VAL
2	C	133	THR
2	C	142	ASP
2	C	145	THR
2	C	156	GLN
2	C	168	VAL
2	C	180	LEU
2	C	190	VAL
2	C	203	VAL
2	C	207	ASP
2	C	217	THR
2	C	231	LEU
2	C	243	GLN
2	C	244	SER
2	C	248	VAL
2	C	264	LEU
2	C	281	VAL
2	C	285	VAL
2	C	289	THR
2	C	294	VAL

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Mol	Chain	Res	Type
2	C	296	VAL
2	C	305	THR
2	C	315	THR
2	C	318	LEU
2	C	323	THR
2	C	329	LEU
2	C	330	THR
2	C	339	LEU
2	C	340	VAL
2	C	341	LYS
2	C	342	THR
2	C	363	ARG
2	C	375	ARG
2	C	384	MET
2	C	475	ILE
2	C	484	ARG
2	C	489	MET
2	C	508	ILE
2	C	546	VAL
2	C	552	VAL
2	C	579	LEU
2	C	599	THR
2	C	603	ILE
2	C	626	ARG
2	C	633	THR
2	C	637	TYR
2	C	654	THR
2	C	661	ASN
2	C	663	VAL
2	C	664	ASN
2	C	674	LYS
2	C	678	SER
2	C	684	LEU
2	C	696	VAL
2	C	701	HIS
2	C	708	THR
2	C	710	SER
2	C	713	MET
2	C	760	THR
2	C	767	LEU
2	C	775	VAL
2	C	815	LEU

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Mol	Chain	Res	Type
2	C	820	ILE
2	C	828	ASP
2	C	833	ARG
2	C	851	THR
2	C	865	ILE
2	C	892	VAL
2	C	896	LEU
2	C	911	ARG
2	C	946	LEU
2	C	962	ASP
2	C	980	ARG
2	C	1005	LEU
2	C	1009	THR
2	C	1014	MET
2	C	1016	ASN
2	C	1027	THR
2	C	1029	LEU
2	C	1035	ILE
2	C	1052	LEU
2	C	1055	LEU
2	C	1056	SER
2	C	1060	ARG
2	C	1061	LEU
2	C	1069	ARG
2	C	1070	ARG
2	C	1072	ASN
2	C	1079	LEU
2	C	1092	VAL
2	C	1116	ARG
2	C	1138	HIS
2	C	1163	ASN
2	C	1188	VAL
2	C	1201	LEU
2	C	1202	PHE
2	C	1225	GLU
2	C	1230	ILE
2	C	1233	LEU
2	C	1251	VAL
2	C	1267	THR
2	C	1269	THR
2	C	1320	VAL
2	C	1331	ARG

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Mol	Chain	Res	Type
3	D	2	LEU
3	D	21	ASN
3	D	29	THR
3	D	30	GLN
3	D	47	LYS
3	D	51	THR
3	D	70	ASP
3	D	73	THR
3	D	77	PHE
3	D	92	ARG
3	D	93	LEU
3	D	116	THR
3	D	133	THR
3	D	139	ASN
3	D	142	THR
3	D	149	MET
3	D	158	LEU
3	D	160	LEU
3	D	191	ARG
3	D	226	MET
3	D	240	VAL
3	D	252	LEU
3	D	266	THR
3	D	273	LEU
3	D	281	LYS
3	E	2	LEU
3	E	29	THR
3	E	48	THR
3	E	54	THR
3	E	66	VAL
3	E	92	ARG
3	E	93	LEU
3	E	116	THR
3	E	133	THR
3	E	139	ASN
3	E	160	LEU
3	E	189	LEU
3	E	213	LEU
3	E	226	MET
3	E	252	LEU
3	E	257	VAL
3	E	262	THR

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Mol	Chain	Res	Type
3	E	272	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	208	HIS
1	A	286	ASN
1	A	595	ASN
1	A	910	ASN
2	B	491	ASN
2	B	526	ASN
2	B	858	HIS
2	B	1138	HIS
2	C	156	GLN
2	C	293	ASN
2	C	430	ASN
2	C	526	ASN
2	C	724	HIS
2	C	981	HIS
2	C	1138	HIS
2	C	1186	GLN
2	C	1203	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	SAM	A	1101	-	23,29,29	1.06	2 (8%)	15,42,42	2.92	2 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SAM	A	1101	-	-	0/8/33/33	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1101	SAM	C2-N1	2.53	1.38	1.33
4	A	1101	SAM	C2-N3	3.47	1.38	1.32

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1101	SAM	N3-C2-N1	-10.65	120.51	128.87
4	A	1101	SAM	C4'-O4'-C1'	2.14	111.91	109.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1101	SAM	5	0

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.