



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Oct 28, 2019 – 03:28 PM EDT

PDB ID : 6ACD
EMDB ID: : EMD-9589
Title : Trypsin-cleaved and low pH-treated SARS-CoV spike glycoprotein and ACE2 complex, ACE2-free conformation with one RBD in up conformation
Authors : Gui, M.; Song, W.
Deposited on : 2018-07-26
Resolution : 3.90 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

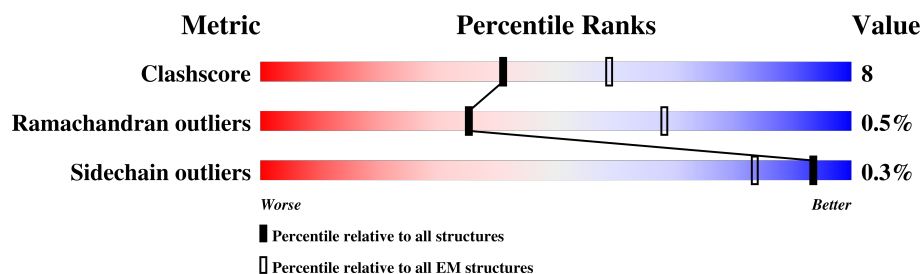
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 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	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

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	1203	71% 17% • 11%
1	B	1203	69% 19% 11%
1	C	1203	69% 18% • 12%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 24845 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1065	Total	C	N	O	S	0	0
			8302	5304	1374	1579	45		
1	B	1065	Total	C	N	O	S	0	0
			8302	5304	1374	1579	45		
1	C	1057	Total	C	N	O	S	0	0
			8241	5264	1364	1568	45		

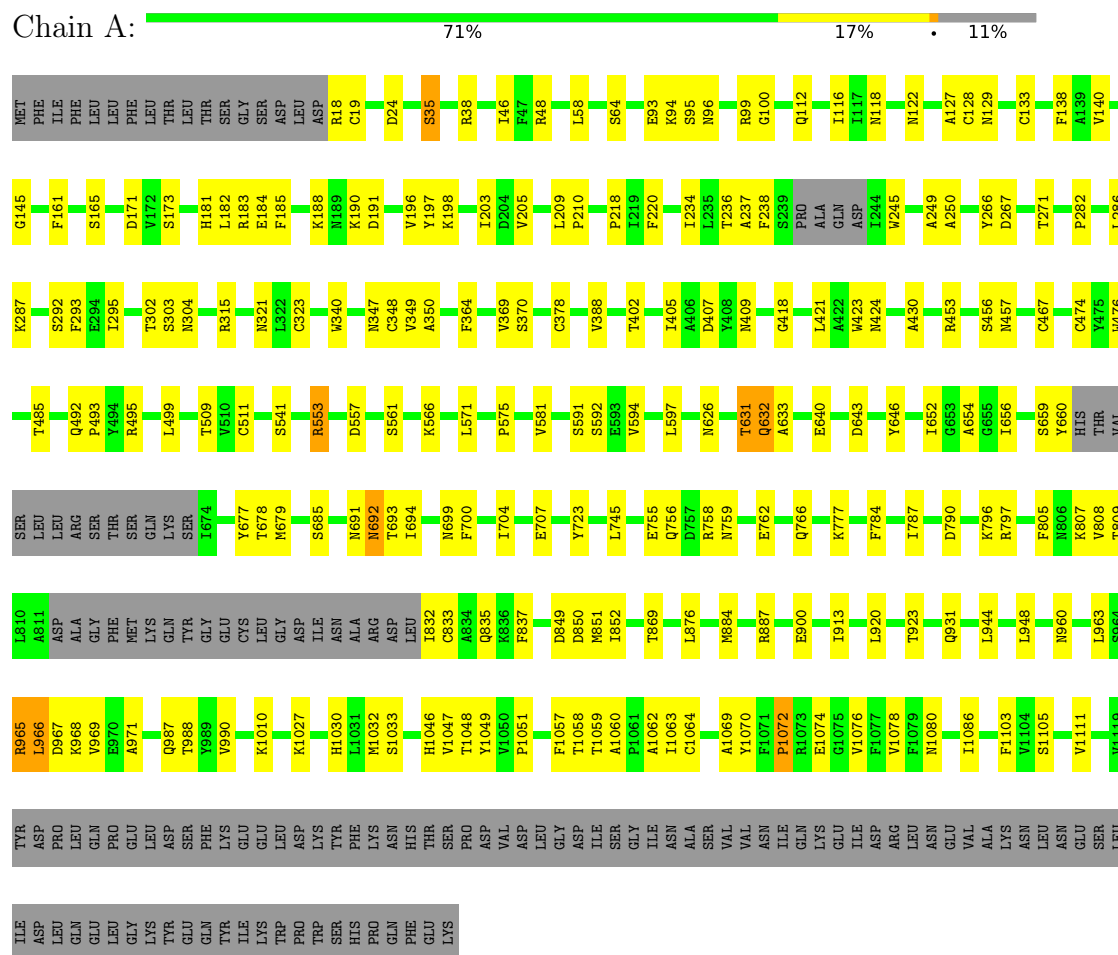
There are 21 discrepancies between the modelled and reference sequences:

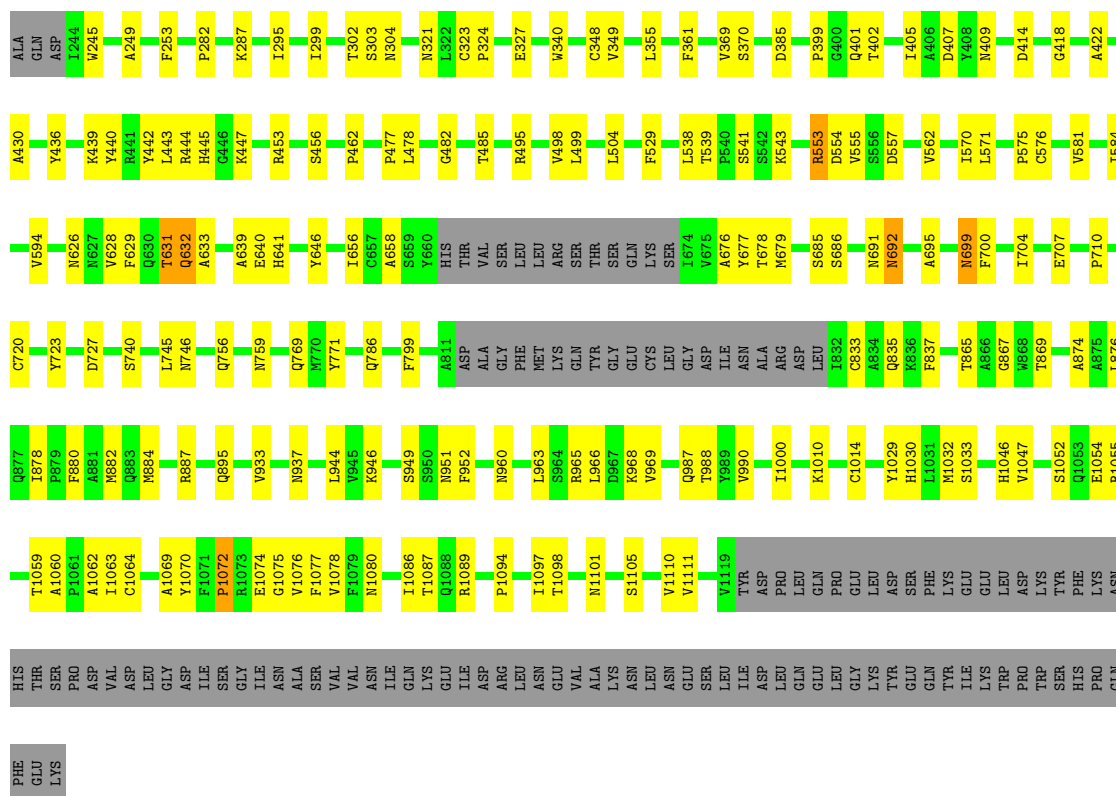
Chain	Residue	Modelled	Actual	Comment	Reference
A	1197	SER	-	expression tag	UNP P59594
A	1198	HIS	-	expression tag	UNP P59594
A	1199	PRO	-	expression tag	UNP P59594
A	1200	GLN	-	expression tag	UNP P59594
A	1201	PHE	-	expression tag	UNP P59594
A	1202	GLU	-	expression tag	UNP P59594
A	1203	LYS	-	expression tag	UNP P59594
B	1197	SER	-	expression tag	UNP P59594
B	1198	HIS	-	expression tag	UNP P59594
B	1199	PRO	-	expression tag	UNP P59594
B	1200	GLN	-	expression tag	UNP P59594
B	1201	PHE	-	expression tag	UNP P59594
B	1202	GLU	-	expression tag	UNP P59594
B	1203	LYS	-	expression tag	UNP P59594
C	1197	SER	-	expression tag	UNP P59594
C	1198	HIS	-	expression tag	UNP P59594
C	1199	PRO	-	expression tag	UNP P59594
C	1200	GLN	-	expression tag	UNP P59594
C	1201	PHE	-	expression tag	UNP P59594
C	1202	GLU	-	expression tag	UNP P59594
C	1203	LYS	-	expression tag	UNP P59594

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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.

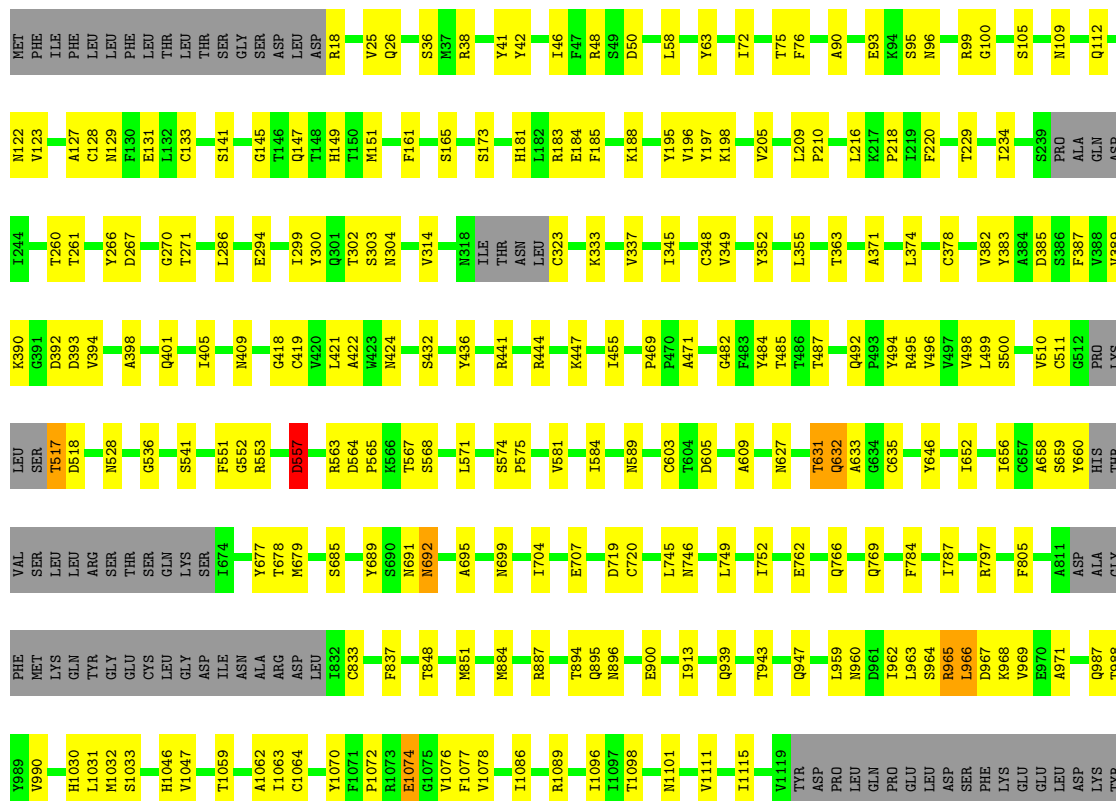
• Molecule 1: Spike glycoprotein





• Molecule 1: Spike glycoprotein

Chain C: 69% 18% 12%



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

HIS
PRO
GLN
PHE
GLU
LYS

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	174489	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.38	0/8499	0.60	2/11568 (0.0%)
1	B	0.38	0/8499	0.60	3/11568 (0.0%)
1	C	0.38	0/8435	0.61	5/11477 (0.0%)
All	All	0.38	0/25433	0.60	10/34613 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	7
1	C	0	3
All	All	0	15

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	557	ASP	CB-CG-OD1	7.57	125.12	118.30
1	C	517	THR	N-CA-C	7.50	131.24	111.00
1	A	966	LEU	CA-CB-CG	6.75	130.83	115.30
1	B	557	ASP	CB-CG-OD1	6.70	124.33	118.30
1	B	966	LEU	CA-CB-CG	6.18	129.52	115.30
1	C	557	ASP	CB-CG-OD1	5.64	123.37	118.30
1	C	966	LEU	CA-CB-CG	5.38	127.67	115.30
1	C	517	THR	C-N-CA	-5.29	108.48	121.70
1	B	504	LEU	CA-CB-CG	5.07	126.95	115.30
1	C	517	THR	CB-CA-C	-5.02	98.06	111.60

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1074	GLU	Peptide
1	A	35	SER	Peptide
1	A	553	ARG	Peptide
1	A	631	THR	Peptide
1	A	923	THR	Peptide
1	B	1052	SER	Peptide
1	B	1074	GLU	Peptide
1	B	1077	PHE	Peptide
1	B	553	ARG	Peptide
1	B	629	PHE	Peptide
1	B	631	THR	Peptide
1	B	727	ASP	Peptide
1	C	1074	GLU	Peptide
1	C	1077	PHE	Peptide
1	C	631	THR	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8302	0	8082	136	0
1	B	8302	0	8082	143	0
1	C	8241	0	8009	154	0
All	All	24845	0	24173	395	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 8.

All (395) 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:C:418:GLY:HA3	1:C:499:LEU:O	1.61	1.00
1:C:314:VAL:H	1:C:517:THR:HG21	1.29	0.96
1:A:100:GLY:HA2	1:A:116:ILE:O	1.68	0.92
1:B:18:ARG:N	1:B:133:CYS:HG	1.66	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:GLU:O	1:C:181:HIS:HB2	1.77	0.84
1:B:1069:ALA:HB3	1:B:1105:SER:O	1.77	0.84
1:A:418:GLY:HA3	1:A:499:LEU:O	1.83	0.79
1:A:1069:ALA:HB3	1:A:1105:SER:O	1.87	0.74
1:C:18:ARG:N	1:C:133:CYS:HG	1.86	0.73
1:C:692:ASN:HB3	1:C:1059:THR:H	1.53	0.73
1:A:18:ARG:N	1:A:133:CYS:HG	1.87	0.71
1:B:740:SER:H	1:C:947:GLN:HE22	1.39	0.71
1:C:419:CYS:O	1:C:498:VAL:HA	1.91	0.71
1:B:692:ASN:HB3	1:B:1059:THR:H	1.56	0.70
1:C:383:TYR:HB2	1:C:500:SER:HB2	1.73	0.70
1:C:314:VAL:N	1:C:517:THR:HG21	1.95	0.69
1:A:405:ILE:HG23	1:A:409:ASN:HD22	1.55	0.69
1:C:405:ILE:HG23	1:C:409:ASN:HD22	1.58	0.68
1:C:536:GLY:HA3	1:C:574:SER:HA	1.75	0.67
1:C:390:LYS:HE3	1:C:392:ASP:HB2	1.75	0.67
1:A:685:SER:HB2	1:C:769:GLN:HE21	1.60	0.65
1:B:348:CYS:SG	1:B:349:VAL:N	2.70	0.65
1:C:960:ASN:H	1:C:963:LEU:HD13	1.62	0.64
1:B:405:ILE:HG23	1:B:409:ASN:HD22	1.60	0.64
1:A:1072:PRO:HB3	1:A:1086:ILE:HD13	1.80	0.63
1:A:745:LEU:HD22	1:A:990:VAL:HG21	1.80	0.63
1:B:340:TRP:O	1:B:453:ARG:NH1	2.30	0.63
1:B:987:GLN:NE2	1:C:988:THR:OG1	2.31	0.63
1:B:385:ASP:HB2	1:B:498:VAL:HB	1.79	0.63
1:C:314:VAL:HG13	1:C:528:ASN:HB3	1.81	0.62
1:A:960:ASN:H	1:A:963:LEU:HD13	1.65	0.62
1:B:302:THR:HG23	1:B:581:VAL:HG23	1.82	0.62
1:C:1078:VAL:HA	1:C:1086:ILE:HG12	1.80	0.62
1:A:347:ASN:H	1:A:509:THR:HB	1.65	0.62
1:A:58:LEU:HB2	1:A:188:LYS:HE3	1.81	0.62
1:C:99:ARG:HD2	1:C:147:GLN:HE22	1.65	0.61
1:A:369:VAL:HA	1:C:965:ARG:HB2	1.81	0.61
1:B:626:ASN:ND2	1:B:639:ALA:O	2.33	0.61
1:A:140:VAL:HG13	1:A:145:GLY:HA2	1.81	0.61
1:A:707:GLU:OE1	1:A:1046:HIS:NE2	2.33	0.61
1:C:887:ARG:NH1	1:C:1032:MET:SD	2.74	0.61
1:B:869:THR:OG1	1:C:1089:ARG:NH1	2.33	0.61
1:B:887:ARG:NH1	1:B:1032:MET:SD	2.73	0.61
1:A:128:CYS:SG	1:A:129:ASN:N	2.74	0.61
1:A:348:CYS:SG	1:A:349:VAL:N	2.74	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:444:ARG:NH1	1:B:447:LYS:O	2.34	0.60
1:C:127:ALA:HB3	1:C:161:PHE:HB3	1.82	0.60
1:B:745:LEU:HD22	1:B:990:VAL:HG21	1.84	0.60
1:C:652:ILE:HD11	1:C:658:ALA:HB2	1.83	0.60
1:A:692:ASN:HB3	1:A:1059:THR:H	1.67	0.60
1:A:887:ARG:NH1	1:A:1032:MET:SD	2.75	0.60
1:C:196:VAL:HB	1:C:220:PHE:HB2	1.83	0.60
1:B:91:ALA:HB3	1:B:183:ARG:HB2	1.83	0.60
1:B:94:LYS:HB3	1:B:175:LYS:HB2	1.82	0.60
1:B:418:GLY:HA3	1:B:499:LEU:O	2.02	0.59
1:B:833:CYS:SG	1:C:632:GLN:NE2	2.75	0.59
1:C:128:CYS:SG	1:C:129:ASN:N	2.75	0.59
1:C:50:ASP:HA	1:C:266:TYR:O	2.03	0.59
1:A:988:THR:OG1	1:C:987:GLN:NE2	2.35	0.59
1:C:149:HIS:NE2	1:C:151:MET:SD	2.76	0.59
1:B:769:GLN:HE21	1:C:685:SER:HB2	1.67	0.59
1:C:564:ASP:HB3	1:C:568:SER:HB3	1.84	0.59
1:A:869:THR:OG1	1:B:1089:ARG:NH1	2.36	0.59
1:A:851:MET:N	1:A:851:MET:SD	2.76	0.58
1:B:47:PHE:HB3	1:C:552:GLY:HA2	1.85	0.58
1:B:1064:CYS:HB2	1:B:1111:VAL:HG11	1.83	0.58
1:A:632:GLN:NE2	1:C:833:CYS:SG	2.76	0.58
1:B:707:GLU:OE2	1:B:1010:LYS:NZ	2.36	0.58
1:C:1096:ILE:O	1:C:1101:ASN:ND2	2.37	0.58
1:B:188:LYS:HB3	1:B:195:TYR:HB2	1.85	0.58
1:B:707:GLU:OE1	1:B:1046:HIS:NE2	2.37	0.58
1:B:99:ARG:NH2	1:B:171:ASP:O	2.36	0.57
1:C:302:THR:HG23	1:C:581:VAL:HG23	1.85	0.57
1:B:835:GLN:HG2	1:C:575:PRO:HG2	1.87	0.57
1:A:302:THR:HG23	1:A:581:VAL:HG23	1.87	0.57
1:B:25:VAL:HA	1:B:76:PHE:HB3	1.86	0.57
1:A:1078:VAL:HA	1:A:1086:ILE:HG12	1.87	0.57
1:A:700:PHE:HA	1:A:1051:PRO:HA	1.87	0.57
1:B:1063:ILE:HB	1:B:1070:TYR:HB2	1.86	0.57
1:B:324:PRO:O	1:B:327:GLU:HB3	2.04	0.56
1:C:141:SER:HB3	1:C:145:GLY:H	1.70	0.56
1:A:138:PHE:HB2	1:A:236:THR:HA	1.87	0.56
1:C:1063:ILE:HB	1:C:1070:TYR:HB2	1.87	0.56
1:C:1064:CYS:HB2	1:C:1111:VAL:HG11	1.87	0.56
1:A:575:PRO:HD3	1:C:837:PHE:HB3	1.87	0.56
1:B:867:GLY:HA3	1:B:876:LEU:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:960:ASN:H	1:B:963:LEU:HD13	1.70	0.56
1:B:72:ILE:H	1:B:75:THR:HB	1.70	0.56
1:C:784:PHE:HA	1:C:787:ILE:HD12	1.86	0.56
1:C:1030:HIS:HE1	1:C:1033:SER:HB2	1.70	0.56
1:C:707:GLU:OE1	1:C:1046:HIS:NE2	2.39	0.56
1:B:120:SER:HA	1:B:170:LEU:HD23	1.87	0.56
1:A:38:ARG:NH1	1:A:184:GLU:OE2	2.38	0.55
1:C:422:ALA:HA	1:C:495:ARG:O	2.06	0.55
1:B:439:LYS:HD3	1:B:478:LEU:HB3	1.87	0.55
1:C:517:THR:OG1	1:C:518:ASP:N	2.39	0.55
1:B:710:PRO:HB2	1:B:1000:ILE:HD11	1.89	0.55
1:A:96:ASN:HA	1:A:183:ARG:HH12	1.71	0.55
1:A:837:PHE:HB3	1:B:575:PRO:HD3	1.88	0.55
1:C:631:THR:O	1:C:633:ALA:N	2.40	0.55
1:A:99:ARG:HD3	1:A:118:ASN:HB2	1.89	0.55
1:B:90:ALA:HB3	1:B:253:PHE:HB2	1.88	0.55
1:A:99:ARG:NH2	1:A:171:ASP:O	2.38	0.54
1:A:24:ASP:HB3	1:A:245:TRP:HE1	1.72	0.54
1:B:72:ILE:HG13	1:B:74:HIS:H	1.72	0.54
1:B:445:HIS:HE1	1:B:462:PRO:HA	1.72	0.54
1:A:631:THR:HB	1:A:654:ALA:HB3	1.90	0.54
1:A:707:GLU:OE2	1:A:1010:LYS:NZ	2.33	0.54
1:A:900:GLU:HA	1:B:1110:VAL:HG11	1.89	0.54
1:A:456:SER:HB2	1:C:112:GLN:HE22	1.72	0.54
1:C:260:THR:OG1	1:C:261:THR:N	2.41	0.54
1:A:755:GLU:OE2	1:A:758:ARG:NH1	2.40	0.54
1:B:1078:VAL:HA	1:B:1086:ILE:HG12	1.88	0.54
1:A:424:ASN:ND2	1:A:492:GLN:OE1	2.40	0.54
1:C:42:TYR:HB2	1:C:218:PRO:HD3	1.90	0.54
1:C:1062:ALA:HB3	1:C:1111:VAL:HG13	1.90	0.53
1:A:777:LYS:NZ	1:A:790:ASP:OD1	2.41	0.53
1:B:116:ILE:HG12	1:B:125:ILE:HG12	1.90	0.53
1:B:402:THR:HB	1:B:407:ASP:HB2	1.91	0.53
1:C:517:THR:O	1:C:517:THR:HG23	2.07	0.53
1:B:99:ARG:HD3	1:B:118:ASN:HB2	1.91	0.52
1:C:960:ASN:HA	1:C:963:LEU:HB2	1.92	0.52
1:A:315:ARG:HH22	1:A:566:LYS:HD2	1.74	0.52
1:C:48:ARG:HB2	1:C:266:TYR:HD2	1.74	0.52
1:A:196:VAL:HB	1:A:220:PHE:HB2	1.90	0.52
1:C:299:ILE:HG12	1:C:584:ILE:HG13	1.90	0.52
1:C:424:ASN:ND2	1:C:492:GLN:OE1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:TRP:O	1:A:453:ARG:NH1	2.43	0.52
1:C:966:LEU:HB2	1:C:971:ALA:HB2	1.90	0.52
1:C:209:LEU:HD12	1:C:210:PRO:HD2	1.92	0.52
1:C:36:SER:HA	1:C:63:TYR:H	1.75	0.52
1:C:96:ASN:HA	1:C:183:ARG:HH12	1.75	0.52
1:A:808:VAL:HA	1:A:931:GLN:HE21	1.73	0.52
1:A:1060:ALA:HB2	1:A:1080:ASN:HD22	1.74	0.52
1:B:756:GLN:HA	1:B:759:ASN:HD22	1.75	0.52
1:A:190:LYS:NZ	1:A:191:ASP:OD2	2.42	0.52
1:A:704:ILE:HG12	1:A:1047:VAL:HG22	1.92	0.52
1:C:100:GLY:HA3	1:C:234:ILE:HB	1.90	0.52
1:B:100:GLY:HA2	1:B:117:ILE:HG22	1.92	0.52
1:C:541:SER:HA	1:C:571:LEU:HG	1.92	0.52
1:A:631:THR:O	1:A:633:ALA:N	2.42	0.51
1:C:887:ARG:NH1	1:C:1031:LEU:O	2.40	0.51
1:C:968:LYS:HG3	1:C:969:VAL:HG23	1.92	0.51
1:A:1062:ALA:HB3	1:A:1111:VAL:HG13	1.92	0.51
1:A:35:SER:OG	1:A:64:SER:N	2.42	0.51
1:C:38:ARG:NH1	1:C:184:GLU:OE2	2.43	0.51
1:C:385:ASP:HB2	1:C:498:VAL:HB	1.92	0.51
1:B:47:PHE:N	1:C:551:PHE:O	2.40	0.51
1:A:323:CYS:N	1:A:348:CYS:SG	2.84	0.51
1:B:24:ASP:HB3	1:B:245:TRP:HE1	1.76	0.51
1:B:190:LYS:O	1:B:193:PHE:HB2	2.11	0.50
1:B:95:SER:OG	1:B:173:SER:O	2.28	0.50
1:B:78:ASN:O	1:B:232:ARG:NH2	2.44	0.50
1:A:835:GLN:NE2	1:B:575:PRO:O	2.43	0.50
1:A:553:ARG:HD2	1:C:46:ILE:HG21	1.92	0.50
1:C:432:SER:HA	1:C:485:THR:H	1.75	0.50
1:A:1103:PHE:HE2	1:C:896:ASN:HD21	1.60	0.50
1:A:1063:ILE:HB	1:A:1070:TYR:HB2	1.94	0.50
1:B:1087:THR:HG22	1:B:1094:PRO:HA	1.94	0.50
1:B:678:THR:OG1	1:B:679:MET:N	2.43	0.50
1:C:363:THR:O	1:C:421:LEU:HA	2.12	0.50
1:C:441:ARG:NH2	1:C:455:ILE:O	2.45	0.50
1:B:127:ALA:HB3	1:B:161:PHE:HB3	1.94	0.50
1:C:185:PHE:HE1	1:C:198:LYS:HG3	1.77	0.50
1:B:538:LEU:HD22	1:B:570:ILE:HD12	1.93	0.50
1:A:94:LYS:NZ	1:A:249:ALA:O	2.39	0.50
1:B:302:THR:OG1	1:B:303:SER:N	2.43	0.50
1:A:321:ASN:HB3	1:A:348:CYS:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:762:GLU:O	1:C:766:GLN:NE2	2.38	0.50
1:C:896:ASN:O	1:C:900:GLU:HB2	2.12	0.50
1:B:631:THR:O	1:B:633:ALA:N	2.40	0.49
1:B:884:MET:HA	1:B:887:ARG:HB2	1.94	0.49
1:A:282:PRO:HB2	1:A:594:VAL:HG21	1.94	0.49
1:B:529:PHE:HE2	1:B:562:VAL:HG21	1.77	0.49
1:B:539:THR:HG23	1:B:571:LEU:HB2	1.94	0.49
1:C:1098:THR:H	1:C:1101:ASN:HB2	1.77	0.49
1:B:1030:HIS:HE1	1:B:1033:SER:HB2	1.76	0.49
1:B:626:ASN:ND2	1:B:640:GLU:OE2	2.45	0.49
1:C:337:VAL:HG22	1:C:387:PHE:HB2	1.95	0.49
1:B:282:PRO:HB2	1:B:594:VAL:HG21	1.94	0.49
1:C:745:LEU:HD22	1:C:990:VAL:HG21	1.93	0.49
1:C:968:LYS:HG3	1:C:969:VAL:H	1.77	0.49
1:B:436:TYR:HE1	1:B:482:GLY:HA2	1.77	0.49
1:B:115:ILE:O	1:B:125:ILE:HA	2.13	0.48
1:B:133:CYS:HB2	1:B:136:PRO:HD3	1.94	0.48
1:A:304:ASN:ND2	1:C:719:ASP:OD1	2.46	0.48
1:A:678:THR:OG1	1:A:679:MET:N	2.40	0.48
1:B:141:SER:HB3	1:B:144:MET:HB2	1.93	0.48
1:B:78:ASN:ND2	1:B:233:ALA:O	2.45	0.48
1:A:185:PHE:HE1	1:A:198:LYS:HG3	1.79	0.48
1:B:105:SER:O	1:B:229:THR:OG1	2.30	0.48
1:A:966:LEU:HB2	1:A:971:ALA:HB2	1.94	0.48
1:C:95:SER:H	1:C:181:HIS:CD2	2.32	0.48
1:C:323:CYS:SG	1:C:349:VAL:N	2.86	0.48
1:B:835:GLN:NE2	1:C:575:PRO:O	2.39	0.48
1:A:626:ASN:ND2	1:A:640:GLU:OE2	2.38	0.48
1:A:659:SER:OG	1:A:660:TYR:N	2.47	0.48
1:C:720:CYS:SG	1:C:746:ASN:ND2	2.87	0.48
1:B:771:TYR:OH	1:B:874:ALA:O	2.31	0.48
1:C:363:THR:HB	1:C:422:ALA:HB3	1.95	0.48
1:A:960:ASN:HA	1:A:963:LEU:HB2	1.95	0.48
1:A:402:THR:HB	1:A:407:ASP:HB2	1.95	0.48
1:A:1064:CYS:HB2	1:A:1111:VAL:HG21	1.96	0.48
1:A:182:LEU:HD22	1:A:203:ILE:HD13	1.95	0.48
1:B:443:LEU:HB2	1:B:477:PRO:HB3	1.96	0.48
1:C:848:THR:HB	1:C:851:MET:HG2	1.96	0.47
1:B:704:ILE:HG12	1:B:1047:VAL:HG22	1.96	0.47
1:B:541:SER:HB3	1:B:543:LYS:HG2	1.97	0.47
1:A:140:VAL:O	1:A:238:PHE:HA	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:659:SER:OG	1:C:660:TYR:N	2.47	0.47
1:C:48:ARG:HB2	1:C:266:TYR:CD2	2.50	0.47
1:A:99:ARG:HG3	1:A:138:PHE:HE2	1.80	0.47
1:A:267:ASP:OD1	1:A:271:THR:N	2.44	0.47
1:C:787:ILE:HD11	1:C:913:ILE:HD13	1.97	0.47
1:C:41:TYR:HB3	1:C:216:LEU:HB2	1.97	0.47
1:C:704:ILE:HG12	1:C:1047:VAL:HG22	1.96	0.47
1:A:693:THR:HA	1:A:1058:THR:HA	1.97	0.47
1:A:138:PHE:HB3	1:A:140:VAL:HG23	1.97	0.47
1:C:58:LEU:HB2	1:C:188:LYS:HE3	1.97	0.47
1:A:370:SER:HB3	1:C:967:ASP:HB2	1.97	0.46
1:B:399:PRO:HB3	1:B:414:ASP:HA	1.98	0.46
1:C:95:SER:OG	1:C:173:SER:O	2.26	0.46
1:A:797:ARG:HD2	1:A:805:PHE:HE2	1.79	0.46
1:B:95:SER:H	1:B:181:HIS:CD2	2.33	0.46
1:A:38:ARG:HD2	1:A:209:LEU:HD21	1.98	0.46
1:A:796:LYS:HD2	1:A:850:ASP:HB3	1.96	0.46
1:A:46:ILE:HG21	1:B:553:ARG:HD2	1.98	0.46
1:A:876:LEU:HA	1:B:695:ALA:HB3	1.96	0.46
1:C:72:ILE:HG13	1:C:75:THR:H	1.80	0.46
1:A:19:CYS:HA	1:A:133:CYS:HB3	1.98	0.46
1:A:209:LEU:HD12	1:A:210:PRO:HD2	1.97	0.46
1:B:321:ASN:HB3	1:B:348:CYS:HA	1.98	0.46
1:A:968:LYS:HG3	1:A:969:VAL:HG23	1.97	0.46
1:B:554:ASP:OD1	1:B:555:VAL:N	2.49	0.46
1:C:294:GLU:OE2	1:C:589:ASN:ND2	2.42	0.46
1:A:388:VAL:HG22	1:A:495:ARG:HG2	1.98	0.46
1:B:128:CYS:SG	1:B:129:ASN:N	2.88	0.46
1:A:127:ALA:HB3	1:A:161:PHE:HB3	1.98	0.46
1:B:968:LYS:HG3	1:B:969:VAL:H	1.80	0.46
1:A:378:CYS:HA	1:A:511:CYS:HA	1.98	0.46
1:A:787:ILE:HD11	1:A:913:ILE:HD13	1.98	0.46
1:A:561:SER:HA	1:A:571:LEU:HA	1.97	0.45
1:A:835:GLN:NE2	1:B:576:CYS:O	2.49	0.45
1:B:1060:ALA:HB2	1:B:1080:ASN:HD22	1.80	0.45
1:B:209:LEU:HD12	1:B:210:PRO:HD2	1.97	0.45
1:B:878:ILE:HG23	1:B:882:MET:HB2	1.97	0.45
1:C:383:TYR:O	1:C:499:LEU:HA	2.16	0.45
1:C:563:ARG:HH21	1:C:567:THR:HG23	1.81	0.45
1:C:959:LEU:HD23	1:C:962:ILE:HD11	1.96	0.45
1:A:694:ILE:N	1:A:1057:PHE:O	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:378:CYS:HA	1:C:511:CYS:HA	1.98	0.45
1:A:95:SER:OG	1:A:173:SER:O	2.24	0.45
1:A:430:ALA:O	1:A:485:THR:OG1	2.31	0.45
1:C:749:LEU:HD23	1:C:752:ILE:HD12	1.98	0.45
1:B:96:ASN:HA	1:B:183:ARG:HH12	1.81	0.45
1:A:832:ILE:O	1:B:632:GLN:NE2	2.49	0.45
1:C:603:CYS:SG	1:C:627:ASN:ND2	2.82	0.45
1:C:348:CYS:HB3	1:C:510:VAL:HB	1.99	0.45
1:C:26:GLN:HB2	1:C:75:THR:HA	1.99	0.45
1:A:1027:LYS:H	1:A:1048:THR:HG21	1.82	0.45
1:A:597:LEU:HD22	1:A:652:ILE:HG23	1.97	0.45
1:B:401:GLN:HE21	1:C:968:LYS:HG2	1.82	0.45
1:B:837:PHE:HB3	1:C:575:PRO:HD3	1.98	0.45
1:C:95:SER:H	1:C:181:HIS:HD2	1.63	0.45
1:C:25:VAL:HA	1:C:76:PHE:HB3	1.98	0.45
1:C:345:ILE:HB	1:C:382:VAL:HG23	1.98	0.44
1:B:699:ASN:HD22	1:B:700:PHE:H	1.64	0.44
1:C:444:ARG:NH1	1:C:447:LYS:O	2.50	0.44
1:C:894:THR:OG1	1:C:895:GLN:N	2.51	0.44
1:C:371:ALA:HA	1:C:374:LEU:HB2	2.00	0.44
1:A:95:SER:H	1:A:181:HIS:CD2	2.35	0.44
1:C:267:ASP:OD1	1:C:271:THR:N	2.40	0.44
1:A:112:GLN:HE22	1:B:456:SER:HB2	1.82	0.44
1:B:968:LYS:HG3	1:B:969:VAL:HG23	2.00	0.44
1:C:939:GLN:O	1:C:943:THR:OG1	2.25	0.44
1:A:205:VAL:HG21	1:A:210:PRO:HD3	2.00	0.44
1:A:292:SER:OG	1:A:293:PHE:N	2.51	0.44
1:A:122:ASN:ND2	1:A:165:SER:O	2.39	0.44
1:B:723:TYR:OH	1:B:944:LEU:O	2.31	0.44
1:C:1063:ILE:HG23	1:C:1115:ILE:HB	1.99	0.44
1:A:364:PHE:HD1	1:A:421:LEU:HD13	1.83	0.43
1:B:1029:TYR:HE2	1:B:1089:ARG:HH22	1.66	0.43
1:C:421:LEU:O	1:C:496:VAL:HA	2.18	0.43
1:B:1062:ALA:HB3	1:B:1111:VAL:HG13	1.99	0.43
1:C:422:ALA:HB2	1:C:496:VAL:HG22	2.00	0.43
1:C:436:TYR:HE1	1:C:482:GLY:HA2	1.83	0.43
1:A:884:MET:HA	1:A:887:ARG:HB2	1.99	0.43
1:B:355:LEU:HA	1:B:361:PHE:HE2	1.84	0.43
1:C:90:ALA:HA	1:C:183:ARG:O	2.18	0.43
1:B:25:VAL:HG13	1:B:76:PHE:HD2	1.84	0.43
1:B:951:ASN:OD1	1:B:952:PHE:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:603:CYS:N	1:C:635:CYS:SG	2.91	0.43
1:B:876:LEU:HA	1:C:695:ALA:HB3	1.99	0.43
1:A:656:ILE:HA	1:A:678:THR:HA	2.00	0.43
1:A:809:THR:H	1:A:931:GLN:HE21	1.67	0.43
1:B:1014:CYS:HB3	1:B:1030:HIS:CE1	2.53	0.43
1:C:484:TYR:HB2	1:C:487:THR:HG23	2.01	0.43
1:A:467:CYS:HB2	1:A:474:CYS:HB3	1.83	0.43
1:A:965:ARG:HB2	1:B:369:VAL:HA	2.01	0.43
1:A:833:CYS:SG	1:B:632:GLN:NE2	2.90	0.43
1:B:658:ALA:HA	1:B:676:ALA:HA	2.01	0.43
1:C:267:ASP:OD1	1:C:270:GLY:N	2.52	0.43
1:C:286:LEU:HD21	1:C:300:TYR:HD2	1.83	0.43
1:A:430:ALA:HB2	1:A:493:PRO:HG3	1.99	0.43
1:C:50:ASP:CA	1:C:266:TYR:O	2.67	0.43
1:C:389:VAL:HB	1:C:393:ASP:HB2	2.00	0.43
1:C:605:ASP:O	1:C:609:ALA:CB	2.66	0.43
1:A:457:ASN:HD21	1:A:476:TRP:HD1	1.67	0.43
1:A:784:PHE:HA	1:A:787:ILE:HD12	1.99	0.43
1:B:880:PHE:HB2	1:C:689:TYR:OH	2.19	0.43
1:C:469:PRO:HA	1:C:471:ALA:H	1.83	0.43
1:B:94:LYS:NZ	1:B:249:ALA:O	2.36	0.42
1:C:398:ALA:HB3	1:C:401:GLN:HG3	2.00	0.42
1:C:797:ARG:HD2	1:C:805:PHE:HE2	1.82	0.42
1:C:884:MET:HA	1:C:887:ARG:HB2	2.01	0.42
1:A:541:SER:HA	1:A:571:LEU:HG	2.01	0.42
1:A:762:GLU:O	1:A:766:GLN:NE2	2.43	0.42
1:B:946:LYS:O	1:B:949:SER:OG	2.30	0.42
1:C:652:ILE:HD12	1:C:656:ILE:HG22	2.01	0.42
1:A:756:GLN:HA	1:A:759:ASN:HD22	1.84	0.42
1:B:299:ILE:HG12	1:B:584:ILE:HG13	2.01	0.42
1:C:109:ASN:HA	1:C:131:GLU:HA	2.02	0.42
1:C:564:ASP:N	1:C:568:SER:O	2.41	0.42
1:A:967:ASP:HB2	1:B:370:SER:HB3	2.01	0.42
1:B:720:CYS:SG	1:B:746:ASN:ND2	2.92	0.42
1:C:352:TYR:HD1	1:C:355:LEU:HD12	1.83	0.42
1:B:91:ALA:HB1	1:B:93:GLU:HG2	2.02	0.42
1:A:93:GLU:HA	1:A:250:ALA:HB1	2.02	0.42
1:B:1097:ILE:HA	1:B:1101:ASN:HD22	1.84	0.42
1:A:100:GLY:HA3	1:A:234:ILE:HB	2.02	0.42
1:A:287:LYS:HA	1:A:295:ILE:HD11	2.01	0.42
1:B:138:PHE:HE1	1:B:152:ILE:HD11	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:VAL:HB	1:B:220:PHE:HB2	2.02	0.42
1:B:287:LYS:HA	1:B:295:ILE:HD11	2.01	0.42
1:B:786:GLN:HB3	1:B:799:PHE:HB3	2.02	0.42
1:B:933:VAL:O	1:B:937:ASN:ND2	2.52	0.42
1:C:105:SER:O	1:C:229:THR:OG1	2.38	0.42
1:C:302:THR:OG1	1:C:303:SER:N	2.52	0.42
1:A:423:TRP:HE1	1:A:495:ARG:HD2	1.85	0.42
1:B:422:ALA:HA	1:B:495:ARG:O	2.20	0.42
1:B:656:ILE:HA	1:B:678:THR:HA	2.01	0.41
1:C:394:VAL:HG21	1:C:494:TYR:HD2	1.84	0.41
1:A:303:SER:OG	1:A:304:ASN:N	2.54	0.41
1:C:1031:LEU:HD12	1:C:1031:LEU:HA	1.92	0.41
1:C:188:LYS:HB3	1:C:195:TYR:HB2	2.01	0.41
1:A:1030:HIS:HE1	1:A:1033:SER:HB2	1.86	0.41
1:A:237:ALA:HB1	1:A:245:TRP:HA	2.03	0.41
1:B:1098:THR:H	1:B:1101:ASN:HD22	1.69	0.41
1:A:1032:MET:HB2	1:A:1047:VAL:HB	2.02	0.41
1:A:1049:TYR:CE2	1:A:1051:PRO:HG3	2.56	0.41
1:A:643:ASP:N	1:A:643:ASP:OD1	2.54	0.41
1:A:48:ARG:HB2	1:A:266:TYR:CE2	2.55	0.41
1:B:303:SER:OG	1:B:304:ASN:N	2.54	0.41
1:B:646:TYR:HB2	1:B:677:TYR:CZ	2.56	0.41
1:B:122:ASN:OD1	1:B:123:VAL:N	2.53	0.41
1:B:26:GLN:HB2	1:B:75:THR:HA	2.02	0.41
1:C:41:TYR:OH	1:C:188:LYS:NZ	2.48	0.41
1:C:964:SER:OG	1:C:965:ARG:N	2.54	0.41
1:A:96:ASN:HD22	1:A:171:ASP:H	1.69	0.41
1:A:807:LYS:NZ	1:A:920:LEU:O	2.42	0.41
1:B:1072:PRO:HB3	1:B:1086:ILE:HD13	2.01	0.41
1:C:122:ASN:OD1	1:C:123:VAL:N	2.54	0.41
1:A:286:LEU:HG	1:A:295:ILE:HD13	2.03	0.41
1:A:849:ASP:HA	1:A:852:ILE:HD12	2.03	0.41
1:B:187:PHE:HE1	1:B:196:VAL:HG13	1.86	0.41
1:C:678:THR:OG1	1:C:679:MET:N	2.51	0.41
1:A:302:THR:OG1	1:A:303:SER:N	2.51	0.41
1:B:39:GLY:HA3	1:B:60:LEU:HB3	2.03	0.41
1:B:430:ALA:O	1:B:485:THR:OG1	2.36	0.41
1:B:440:TYR:HE2	1:B:442:TYR:HB3	1.86	0.41
1:C:205:VAL:HG21	1:C:210:PRO:HD3	2.03	0.41
1:C:303:SER:OG	1:C:304:ASN:N	2.54	0.40
1:C:564:ASP:HA	1:C:565:PRO:HD3	1.96	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:TYR:CD1	1:A:218:PRO:HA	2.55	0.40
1:A:350:ALA:N	1:A:511:CYS:O	2.52	0.40
1:A:646:TYR:HB2	1:A:677:TYR:CZ	2.56	0.40
1:B:1054:GLU:O	1:B:1055:ARG:NH1	2.53	0.40
1:B:237:ALA:HB1	1:B:245:TRP:HA	2.03	0.40
1:C:197:TYR:CD1	1:C:218:PRO:HA	2.56	0.40
1:C:553:ARG:HD2	1:C:557:ASP:HA	2.02	0.40
1:A:591:SER:OG	1:A:592:SER:N	2.55	0.40
1:B:323:CYS:N	1:B:348:CYS:SG	2.94	0.40
1:B:628:VAL:HG13	1:B:641:HIS:CE1	2.56	0.40
1:C:646:TYR:HB2	1:C:677:TYR:CZ	2.57	0.40
1:A:723:TYR:OH	1:A:944:LEU:O	2.36	0.40
1:A:723:TYR:CZ	1:A:948:LEU:HG	2.56	0.40
1:B:180:LYS:HG3	1:B:202:PRO:HB3	2.02	0.40
1:B:685:SER:OG	1:B:686:SER:N	2.54	0.40
1:B:960:ASN:HA	1:B:963:LEU:HB2	2.03	0.40
1:C:1031:LEU:N	1:C:1047:VAL:O	2.52	0.40
1:C:122:ASN:ND2	1:C:165:SER:O	2.42	0.40
1:A:987:GLN:NE2	1:B:988:THR:OG1	2.55	0.40
1:B:123:VAL:HB	1:B:165:SER:HB3	2.02	0.40
1:B:865:THR:HA	1:C:689:TYR:CE1	2.56	0.40
1:B:895:GLN:HG3	1:C:1074:GLU:HG2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	1057/1203 (88%)	892 (84%)	160 (15%)	5 (0%)	31	71
1	B	1057/1203 (88%)	900 (85%)	151 (14%)	6 (1%)	27	67
1	C	1045/1203 (87%)	897 (86%)	142 (14%)	6 (1%)	27	67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	3159/3609 (88%)	2689 (85%)	453 (14%)	17 (0%)	35	71

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	632	GLN
1	C	632	GLN
1	A	632	GLN
1	A	692	ASN
1	A	1072	PRO
1	B	692	ASN
1	B	1072	PRO
1	C	692	ASN
1	C	1072	PRO
1	A	691	ASN
1	C	557	ASP
1	C	691	ASN
1	B	691	ASN
1	C	1076	VAL
1	B	1075	GLY
1	A	1076	VAL
1	B	1076	VAL

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	922/1048 (88%)	920 (100%)	2 (0%)	94	97
1	B	922/1048 (88%)	920 (100%)	2 (0%)	94	97
1	C	914/1048 (87%)	911 (100%)	3 (0%)	93	96
All	All	2758/3144 (88%)	2751 (100%)	7 (0%)	93	96

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	699	ASN
1	A	965	ARG
1	B	699	ASN
1	B	965	ARG
1	C	333	LYS
1	C	699	ASN
1	C	965	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	GLN
1	A	147	GLN
1	A	149	HIS
1	A	181	HIS
1	A	479	ASN
1	A	632	GLN
1	A	699	ASN
1	A	733	ASN
1	A	759	ASN
1	A	931	GLN
1	A	935	ASN
1	A	942	ASN
1	A	987	GLN
1	A	1030	HIS
1	B	129	ASN
1	B	181	HIS
1	B	304	ASN
1	B	401	GLN
1	B	409	ASN
1	B	445	HIS
1	B	632	GLN
1	B	699	ASN
1	B	759	ASN
1	B	769	GLN
1	B	937	ASN
1	B	984	GLN
1	B	987	GLN
1	B	1030	HIS
1	B	1101	ASN
1	C	147	GLN
1	C	181	HIS
1	C	304	ASN

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Mol	Chain	Res	Type
1	C	632	GLN
1	C	692	ASN
1	C	699	ASN
1	C	769	GLN
1	C	835	GLN
1	C	947	GLN
1	C	984	GLN
1	C	987	GLN
1	C	993	GLN
1	C	1101	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.