



Full wwPDB EM Validation Report ⓘ

May 24, 2026 – 02:14 AM JST

PDB ID : 9VEJ / pdb_00009vej
EMDB ID : EMD-65009
Title : Structural basis for the assembly and translocation of the Vip1-Vip2 insecticidal binary toxin from *Bacillus thuringiensis*
Authors : Chen, P.; Zhao, T.
Deposited on : 2025-06-09
Resolution : 2.40 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : **FAILED**
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

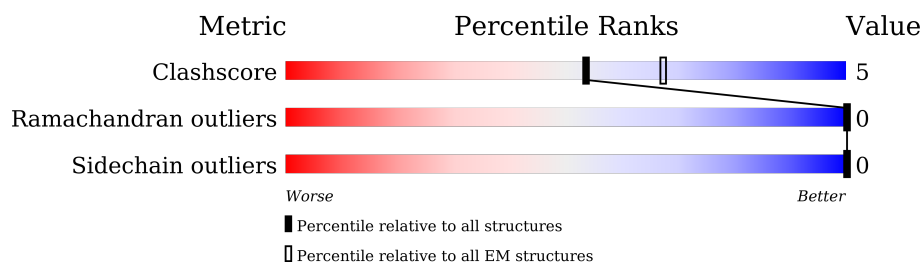
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.40 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	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	656	75% 10% 15%
1	B	656	75% 11% 15%
1	C	656	76% 10% 15%
1	D	656	76% 9% 15%
1	E	656	77% 9% 15%
1	F	656	74% 11% 15%
1	G	656	73% 13% 15%
2	H	390	92% 7%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 33521 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 Vip1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	560	Total	C	N	O	S	0	0
			4344	2710	722	902	10		
1	A	560	Total	C	N	O	S	0	0
			4344	2710	722	902	10		
1	C	560	Total	C	N	O	S	0	0
			4344	2710	722	902	10		
1	D	560	Total	C	N	O	S	0	0
			4344	2710	722	902	10		
1	E	560	Total	C	N	O	S	0	0
			4344	2710	722	902	10		
1	F	560	Total	C	N	O	S	0	0
			4344	2710	722	902	10		
1	G	560	Total	C	N	O	S	0	0
			4344	2710	722	902	10		

- Molecule 2 is a protein called Vip2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	389	Total	C	N	O	S	0	0
			3092	1959	517	604	12		

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
3	B	3	Total	Ca	0
			3	3	
3	A	3	Total	Ca	0
			3	3	
3	C	3	Total	Ca	0
			3	3	
3	D	3	Total	Ca	0
			3	3	

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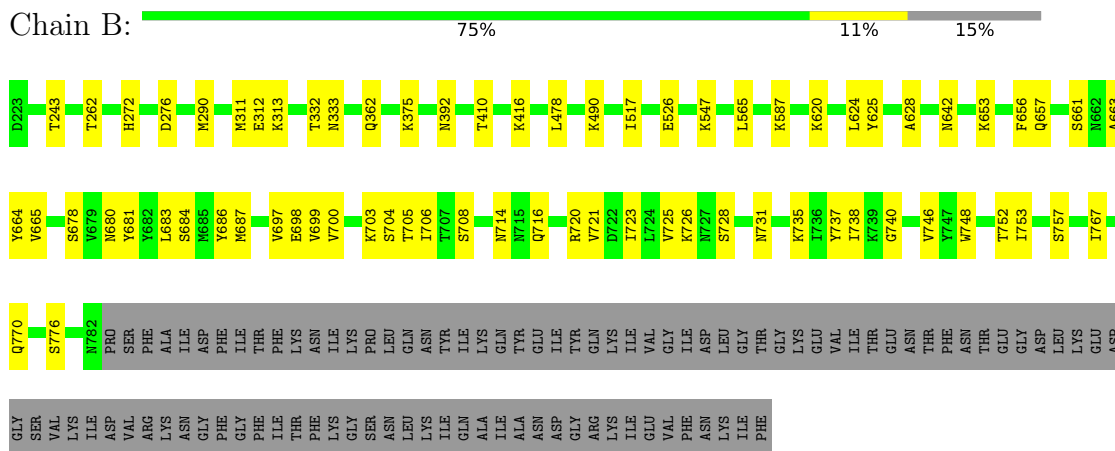
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Mol	Chain	Residues	Atoms		AltConf
3	E	3	Total 3	Ca 3	0
3	F	3	Total 3	Ca 3	0
3	G	3	Total 3	Ca 3	0

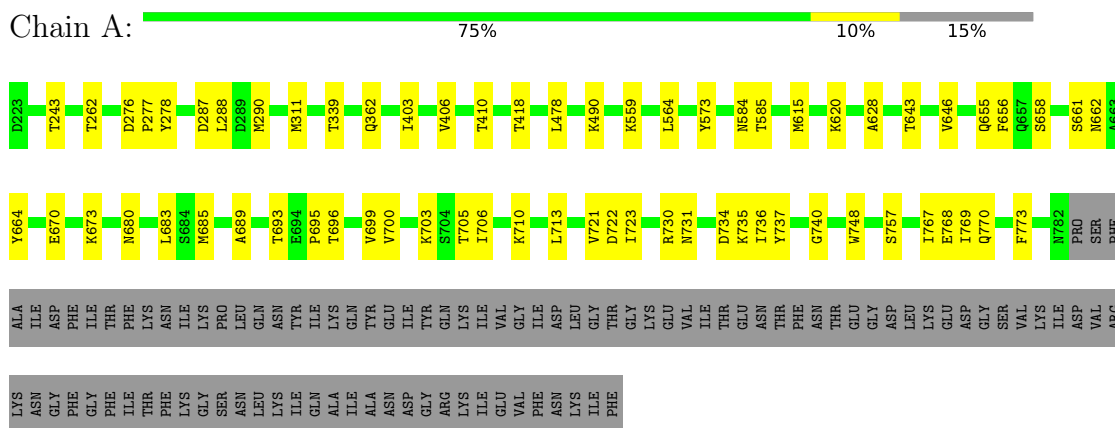
3 Residue-property plots

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

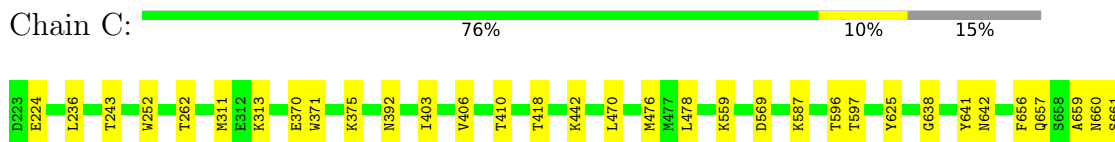
• Molecule 1: Vip1

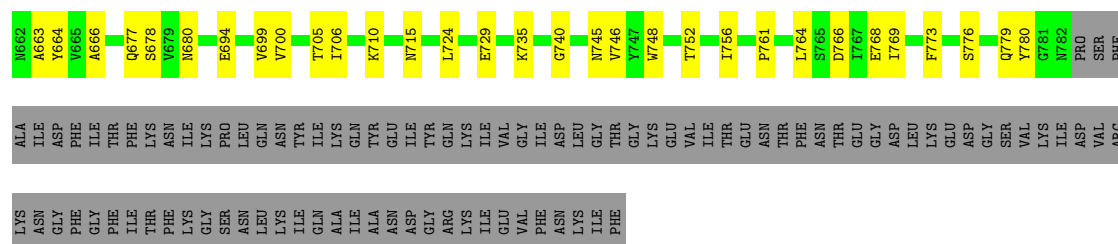


• Molecule 1: Vip1



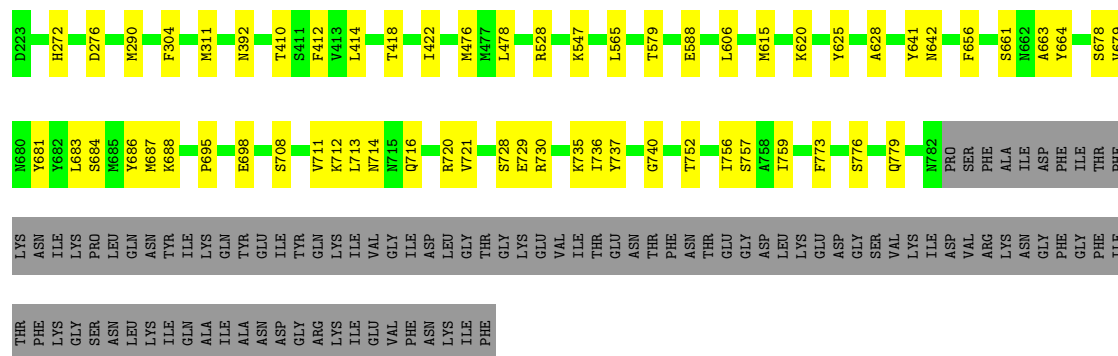
• Molecule 1: Vip1





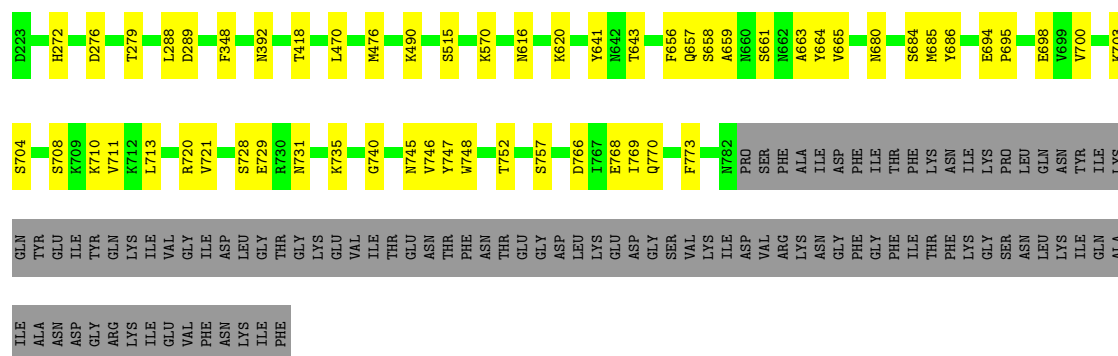
• Molecule 1: Vip1

Chain D: 76% 9% 15%



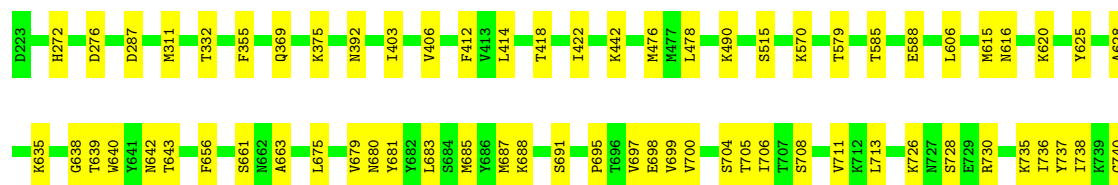
• Molecule 1: Vip1

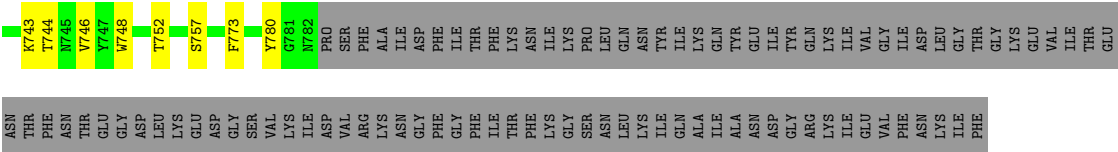
Chain E: 77% 9% 15%



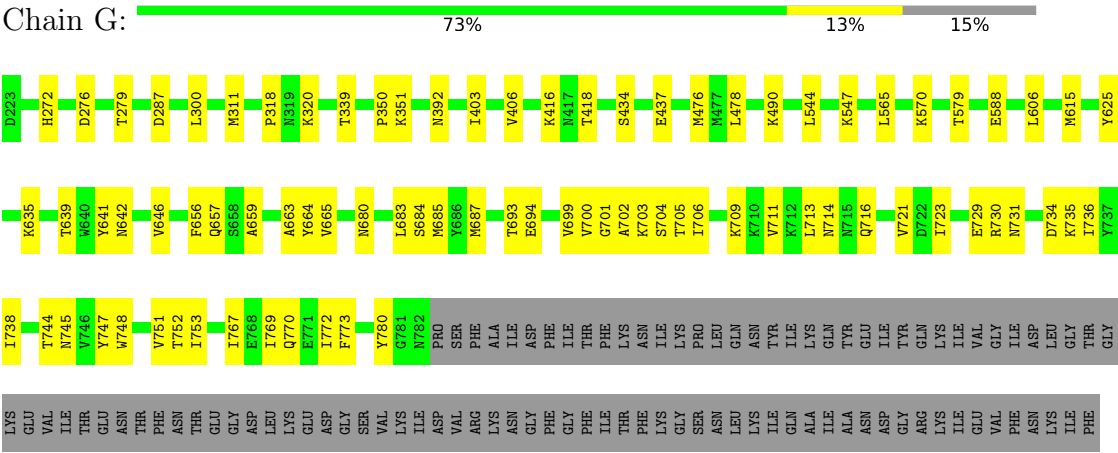
• Molecule 1: Vip1

Chain F: 74% 11% 15%

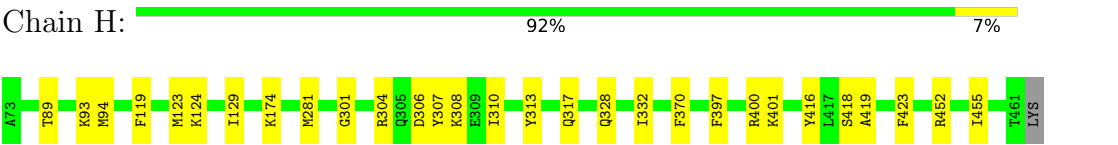




• Molecule 1: Vip1



• Molecule 2: Vip2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	265183	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	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: CA

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	0.21	0/4425	0.36	0/6005
1	B	0.23	0/4425	0.39	0/6005
1	C	0.23	0/4425	0.38	0/6005
1	D	0.21	0/4425	0.36	0/6005
1	E	0.20	0/4425	0.36	0/6005
1	F	0.22	0/4425	0.37	0/6005
1	G	0.21	0/4425	0.38	0/6005
2	H	0.18	0/3144	0.34	0/4220
All	All	0.21	0/34119	0.37	0/46255

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	4344	0	4222	48	0
1	B	4344	0	4222	53	0
1	C	4344	0	4222	45	0
1	D	4344	0	4222	40	0
1	E	4344	0	4222	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	4344	0	4222	57	0
1	G	4344	0	4222	60	0
2	H	3092	0	3113	20	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	3	0	0	0	0
3	E	3	0	0	0	0
3	F	3	0	0	0	0
3	G	3	0	0	0	0
All	All	33521	0	32667	345	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 (345) 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:G:685:MET:HG2	1:G:751:VAL:HG12	1.53	0.91
1:B:311:MET:HE3	1:B:478:LEU:HG	1.60	0.83
1:G:683:LEU:HD12	1:G:753:ILE:HD11	1.62	0.81
1:G:646:VAL:HG11	1:G:747:TYR:CE1	2.16	0.80
1:G:680:ASN:HD21	1:G:770:GLN:HB3	1.48	0.79
1:A:689:ALA:HB1	1:A:693:THR:HG22	1.64	0.79
1:G:700:VAL:HG23	1:G:735:LYS:HG3	1.65	0.77
1:A:695:PRO:HD2	1:A:713:LEU:HD13	1.68	0.76
1:B:664:TYR:HB3	1:B:737:TYR:CD1	2.22	0.75
1:A:693:THR:HG23	1:A:695:PRO:HD3	1.67	0.75
1:F:414:LEU:HB2	1:F:476:MET:HE2	1.68	0.75
1:F:743:LYS:HG3	1:F:744:THR:HG23	1.69	0.75
1:G:700:VAL:HG12	1:G:704:SER:HA	1.69	0.73
1:B:620:LYS:HD3	1:B:757:SER:HB2	1.68	0.73
1:E:620:LYS:HD3	1:E:757:SER:HB2	1.71	0.73
1:G:646:VAL:HG11	1:G:747:TYR:HE1	1.51	0.73
1:E:659:ALA:HB2	1:E:745:ASN:HA	1.71	0.73
1:F:656:PHE:HB2	1:F:748:TRP:CE2	2.24	0.72
1:D:714:ASN:HD22	1:D:716:GLN:HE21	1.38	0.71
1:C:243:THR:HG22	1:C:262:THR:O	1.90	0.70
1:B:680:ASN:HD21	1:B:770:GLN:HB3	1.56	0.70
1:A:735:LYS:HE2	1:A:737:TYR:HE1	1.56	0.70
1:C:694:GLU:HB3	1:C:710:LYS:HE3	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:769:ILE:HD12	1:G:769:ILE:H	1.57	0.69
1:F:705:THR:HG22	1:F:706:ILE:HG23	1.76	0.69
1:D:620:LYS:HD3	1:D:757:SER:HB2	1.76	0.68
1:C:766:ASP:HB3	1:C:769:ILE:HD13	1.78	0.66
1:E:695:PRO:O	1:E:710:LYS:HG3	1.96	0.66
1:F:661:SER:HA	1:F:740:GLY:H	1.61	0.66
1:C:642:ASN:HB2	1:C:663:ALA:HA	1.77	0.66
1:B:681:TYR:HB3	1:B:753:ILE:HD11	1.78	0.65
1:G:625:TYR:HD1	1:G:752:THR:HG22	1.61	0.65
1:D:683:LEU:HD11	1:D:736:ILE:HD12	1.77	0.64
1:B:665:VAL:O	1:B:735:LYS:HA	1.98	0.64
1:F:695:PRO:HD2	1:F:713:LEU:HD13	1.80	0.64
1:F:735:LYS:HE3	1:F:737:TYR:HE1	1.64	0.63
1:A:311:MET:HB2	1:A:478:LEU:HD12	1.81	0.63
1:D:625:TYR:HD1	1:D:752:THR:HG22	1.64	0.62
1:F:699:VAL:HG12	1:F:736:ILE:HG12	1.80	0.62
1:F:700:VAL:HG12	1:F:704:SER:HA	1.78	0.62
1:D:712:LYS:N	1:D:712:LYS:HE2	2.14	0.62
1:F:625:TYR:HD1	1:F:752:THR:HG22	1.64	0.62
1:D:311:MET:HB2	1:D:478:LEU:HD12	1.81	0.62
1:E:700:VAL:HG22	1:E:704:SER:HA	1.81	0.62
1:F:642:ASN:HB2	1:F:663:ALA:HA	1.82	0.61
1:B:706:ILE:HD11	1:B:725:VAL:HG12	1.83	0.61
1:E:694:GLU:HB3	1:E:710:LYS:HD2	1.81	0.61
1:E:728:SER:HB3	1:E:773:PHE:HE1	1.66	0.61
1:D:687:MET:HB3	1:D:713:LEU:HD11	1.83	0.61
1:E:665:VAL:O	1:E:735:LYS:HA	2.01	0.61
1:A:689:ALA:CB	1:A:693:THR:HG22	2.30	0.61
1:E:661:SER:HA	1:E:740:GLY:H	1.66	0.60
2:H:281:MET:HE3	2:H:281:MET:HA	1.83	0.60
1:A:418:THR:H	1:G:392:ASN:HD21	1.48	0.60
1:A:585:THR:HG23	1:A:615:MET:HG2	1.84	0.59
1:A:620:LYS:HD3	1:A:757:SER:HB2	1.84	0.59
1:A:661:SER:HA	1:A:740:GLY:H	1.67	0.59
1:C:243:THR:HG23	1:C:252:TRP:HE3	1.68	0.59
1:A:730:ARG:HG3	1:A:773:PHE:HZ	1.66	0.59
1:F:698:GLU:HB3	1:F:708:SER:HB3	1.85	0.58
1:C:311:MET:HB2	1:C:478:LEU:HD12	1.85	0.58
1:B:517:ILE:HG12	1:B:526:GLU:HG3	1.85	0.58
1:E:515:SER:HB3	1:E:616:ASN:HD22	1.67	0.58
1:G:703:LYS:HE2	1:G:731:ASN:HD21	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:700:VAL:HA	1:C:705:THR:HA	1.85	0.58
2:H:281:MET:HE1	2:H:419:ALA:HA	1.85	0.58
1:C:625:TYR:HD1	1:C:752:THR:HG22	1.66	0.57
1:F:683:LEU:HD11	1:F:736:ILE:HD13	1.86	0.57
1:B:311:MET:CE	1:B:478:LEU:HG	2.34	0.57
1:D:642:ASN:HB2	1:D:663:ALA:HA	1.86	0.57
1:B:333:ASN:HD22	1:C:370:GLU:HB2	1.69	0.56
1:A:656:PHE:HD1	1:A:748:TRP:HE1	1.53	0.56
1:A:656:PHE:HB2	1:A:748:TRP:NE1	2.21	0.56
2:H:119:PHE:O	2:H:123:MET:HG2	2.06	0.56
1:B:699:VAL:HG23	1:B:705:THR:HB	1.87	0.55
1:F:515:SER:HB3	1:F:616:ASN:HD22	1.70	0.55
1:B:392:ASN:HD21	1:C:418:THR:H	1.55	0.55
1:B:642:ASN:HB2	1:B:663:ALA:HA	1.88	0.55
1:D:687:MET:HE1	1:D:711:VAL:HG21	1.87	0.55
1:E:392:ASN:HD21	1:F:418:THR:H	1.54	0.55
2:H:304:ARG:NE	2:H:304:ARG:HA	2.21	0.55
2:H:307:TYR:CE1	2:H:308:LYS:HG3	2.42	0.55
1:A:703:LYS:HB2	1:A:731:ASN:HB3	1.89	0.55
1:B:661:SER:HA	1:B:740:GLY:H	1.72	0.54
1:C:729:GLU:H	1:C:773:PHE:HE2	1.56	0.54
1:A:646:VAL:HG13	1:A:655:GLN:HG3	1.90	0.54
2:H:313:TYR:HA	2:H:317:GLN:HB2	1.90	0.54
1:A:700:VAL:HA	1:A:705:THR:HA	1.89	0.54
1:E:680:ASN:HD21	1:E:770:GLN:HA	1.71	0.54
1:G:729:GLU:HB2	1:G:773:PHE:HE2	1.73	0.53
1:D:730:ARG:HG2	1:D:773:PHE:HZ	1.74	0.53
1:G:730:ARG:HG3	1:G:773:PHE:HZ	1.74	0.53
1:A:699:VAL:HG23	1:A:706:ILE:HB	1.91	0.53
1:E:698:GLU:HB3	1:E:708:SER:HB2	1.91	0.52
1:F:585:THR:HG23	1:F:615:MET:HG2	1.92	0.52
1:E:766:ASP:HB3	1:E:769:ILE:HD13	1.91	0.52
1:F:392:ASN:HD21	1:G:418:THR:H	1.57	0.52
1:E:729:GLU:HB2	1:E:773:PHE:CZ	2.44	0.52
1:B:680:ASN:HD21	1:B:770:GLN:CB	2.21	0.52
1:F:311:MET:HB2	1:F:478:LEU:HD12	1.91	0.52
2:H:89:THR:HG22	2:H:93:LYS:HE2	1.90	0.52
1:F:620:LYS:HD3	1:F:757:SER:HB3	1.92	0.52
1:F:695:PRO:HB3	1:F:740:GLY:HA2	1.90	0.52
1:G:287:ASP:OD1	1:G:490:LYS:HD2	2.10	0.52
1:G:403:ILE:HG12	1:G:406:VAL:HG22	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:696:THR:HG22	1:A:710:LYS:HB3	1.90	0.52
1:C:768:GLU:HG2	1:C:769:ILE:HD12	1.92	0.52
1:B:656:PHE:HB2	1:B:748:TRP:CE2	2.44	0.51
1:B:624:LEU:HB2	1:B:753:ILE:CG2	2.40	0.51
1:A:734:ASP:OD1	1:A:735:LYS:HG2	2.10	0.51
1:E:658:SER:HG	1:E:748:TRP:HH2	1.56	0.51
1:F:680:ASN:ND2	1:F:726:LYS:HD3	2.26	0.51
1:B:628:ALA:HB2	1:B:656:PHE:CE2	2.46	0.51
1:B:700:VAL:HB	1:B:735:LYS:HG3	1.91	0.51
1:F:691:SER:HB2	1:F:744:THR:HG21	1.93	0.51
1:D:414:LEU:HB2	1:D:476:MET:HE2	1.93	0.51
1:C:642:ASN:HB3	1:C:660:ASN:HD22	1.76	0.51
1:G:311:MET:HB2	1:G:478:LEU:HD12	1.93	0.51
1:C:680:ASN:HB2	1:C:756:ILE:CG2	2.41	0.50
1:E:470:LEU:HD21	1:E:476:MET:HE2	1.94	0.50
1:F:412:PHE:HE2	1:F:422:ILE:HD12	1.77	0.50
2:H:416:TYR:CE2	2:H:418:SER:HB2	2.46	0.50
1:A:656:PHE:HB2	1:A:748:TRP:CE2	2.47	0.49
1:D:729:GLU:HB2	1:D:773:PHE:HE2	1.76	0.49
1:G:699:VAL:HG12	1:G:736:ILE:HG23	1.92	0.49
1:B:767:ILE:HB	1:B:770:GLN:HE21	1.76	0.49
1:D:695:PRO:HD2	1:D:713:LEU:HD23	1.94	0.49
1:D:711:VAL:C	1:D:712:LYS:HE2	2.37	0.49
1:F:403:ILE:HG12	1:F:406:VAL:HG22	1.93	0.49
1:B:687:MET:HG2	1:B:748:TRP:HB3	1.95	0.49
1:A:403:ILE:HG12	1:A:406:VAL:HG22	1.94	0.49
1:A:699:VAL:HG12	1:A:736:ILE:HG12	1.95	0.49
1:E:746:VAL:HG12	1:E:747:TYR:N	2.28	0.49
1:A:670:GLU:HA	1:A:673:LYS:HG2	1.95	0.48
1:E:685:MET:HG3	1:E:721:VAL:CG1	2.43	0.48
1:G:702:ALA:HB3	1:G:731:ASN:HD22	1.78	0.48
1:C:761:PRO:HA	1:C:764:LEU:HD12	1.96	0.48
1:G:730:ARG:HG3	1:G:773:PHE:CZ	2.47	0.48
2:H:401:LYS:HA	2:H:452:ARG:HG3	1.94	0.48
1:B:703:LYS:H	1:B:731:ASN:ND2	2.12	0.48
1:E:768:GLU:HG2	1:E:769:ILE:HD12	1.95	0.48
1:D:579:THR:HG21	1:D:606:LEU:HD21	1.95	0.48
1:A:700:VAL:HG13	1:A:735:LYS:HG3	1.96	0.48
1:G:687:MET:HE1	1:G:738:ILE:HD12	1.96	0.48
1:E:656:PHE:HB2	1:E:748:TRP:CE2	2.49	0.48
1:D:779:GLN:HA	1:D:779:GLN:OE1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:679:VAL:HG13	1:F:681:TYR:HE1	1.79	0.48
1:B:687:MET:HE3	1:B:687:MET:HB2	1.66	0.47
1:F:683:LEU:HD11	1:F:736:ILE:CD1	2.44	0.47
1:B:728:SER:HB2	1:B:731:ASN:HB2	1.95	0.47
1:F:588:GLU:HG2	1:F:615:MET:HE3	1.94	0.47
1:B:625:TYR:HD1	1:B:752:THR:HG22	1.78	0.47
1:D:588:GLU:HG2	1:D:615:MET:HE3	1.95	0.47
1:G:547:LYS:HG3	1:G:565:LEU:HD11	1.95	0.47
1:C:715:ASN:OD1	1:C:715:ASN:O	2.33	0.47
1:C:724:LEU:HD23	1:C:766:ASP:HB2	1.97	0.47
1:F:579:THR:HG21	1:F:606:LEU:HD21	1.97	0.47
1:B:678:SER:O	1:B:776:SER:HB3	2.15	0.47
1:C:596:THR:HG23	1:C:597:THR:HG23	1.96	0.47
1:D:661:SER:HA	1:D:740:GLY:H	1.80	0.47
1:G:680:ASN:ND2	1:G:770:GLN:HB3	2.25	0.47
1:G:646:VAL:HB	1:G:657:GLN:HG2	1.96	0.47
1:B:375:LYS:HE2	1:B:375:LYS:HB3	1.64	0.47
1:C:756:ILE:HG23	1:C:779:GLN:NE2	2.30	0.46
1:D:628:ALA:HB2	1:D:656:PHE:CZ	2.50	0.46
2:H:124:LYS:NZ	2:H:124:LYS:HB3	2.30	0.46
2:H:307:TYR:HA	2:H:310:ILE:HG22	1.97	0.46
1:B:332:THR:HG23	1:C:371:TRP:HE3	1.79	0.46
1:G:641:TYR:HD2	1:G:664:TYR:CZ	2.32	0.46
1:G:684:SER:HA	1:G:721:VAL:O	2.15	0.46
1:D:698:GLU:HB2	1:D:708:SER:HB2	1.96	0.46
1:F:679:VAL:HG13	1:F:681:TYR:CE1	2.51	0.46
1:G:767:ILE:HA	1:G:770:GLN:NE2	2.29	0.46
1:G:642:ASN:HB2	1:G:663:ALA:HA	1.98	0.46
2:H:370:PHE:HE2	2:H:455:ILE:HD11	1.80	0.46
1:B:683:LEU:HD22	1:B:723:ILE:HD11	1.97	0.46
1:C:680:ASN:HB2	1:C:756:ILE:HG21	1.97	0.46
1:F:711:VAL:HG23	1:F:713:LEU:HD11	1.98	0.46
2:H:94:MET:HE1	2:H:129:ILE:HG23	1.96	0.46
1:D:678:SER:O	1:D:776:SER:HB3	2.16	0.46
2:H:397:PHE:HB2	2:H:400:ARG:HD2	1.97	0.46
1:B:686:TYR:CZ	1:B:720:ARG:HD2	2.51	0.45
1:A:287:ASP:OD1	1:A:490:LYS:HD2	2.16	0.45
1:D:412:PHE:HE2	1:D:422:ILE:HD12	1.81	0.45
1:B:290:MET:HE3	1:B:290:MET:HB3	1.80	0.45
1:A:768:GLU:HG2	1:A:769:ILE:HD12	1.98	0.45
1:D:628:ALA:HB2	1:D:656:PHE:CE2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:403:ILE:HG12	1:C:406:VAL:HG22	1.98	0.45
1:B:547:LYS:HG3	1:B:565:LEU:HD11	1.99	0.45
1:A:683:LEU:HD12	1:A:723:ILE:HD11	1.99	0.45
1:A:735:LYS:HE2	1:A:737:TYR:CE1	2.42	0.45
1:E:348:PHE:HB2	1:F:355:PHE:HB3	1.97	0.45
1:E:746:VAL:HG12	1:E:747:TYR:H	1.81	0.45
1:F:688:LYS:O	1:F:746:VAL:HG13	2.16	0.45
2:H:328:GLN:O	2:H:332:ILE:HG13	2.17	0.45
1:B:490:LYS:HE3	1:B:490:LYS:HB2	1.78	0.45
1:C:659:ALA:HB2	1:C:745:ASN:HA	1.98	0.45
1:F:570:LYS:HB3	1:F:570:LYS:HE2	1.72	0.45
1:B:680:ASN:ND2	1:B:770:GLN:HB3	2.29	0.45
1:E:657:GLN:HA	1:E:746:VAL:O	2.17	0.45
1:F:728:SER:HB3	1:F:773:PHE:HE2	1.82	0.45
1:G:709:LYS:HG3	1:G:723:ILE:CG2	2.47	0.45
1:B:698:GLU:HB3	1:B:708:SER:HB2	1.98	0.45
1:G:683:LEU:HD12	1:G:753:ILE:CD1	2.41	0.45
1:A:243:THR:HG22	1:A:262:THR:O	2.16	0.44
1:D:686:TYR:CZ	1:D:720:ARG:HD2	2.53	0.44
1:F:656:PHE:HB2	1:F:748:TRP:NE1	2.31	0.44
1:G:588:GLU:HG2	1:G:615:MET:HE3	1.99	0.44
1:G:318:PRO:HB2	1:G:320:LYS:HE2	2.00	0.44
2:H:308:LYS:H	2:H:308:LYS:NZ	2.14	0.44
1:A:767:ILE:HD12	1:A:767:ILE:H	1.82	0.44
1:D:756:ILE:HD12	1:D:759:ILE:HD12	1.98	0.44
1:G:635:LYS:HZ2	1:G:639:THR:HA	1.82	0.44
1:G:646:VAL:HG11	1:G:747:TYR:CD1	2.52	0.44
1:D:290:MET:HE3	1:D:290:MET:HB3	1.87	0.44
1:D:684:SER:HA	1:D:721:VAL:O	2.18	0.44
1:E:643:THR:HA	1:E:658:SER:HB3	1.99	0.44
1:F:698:GLU:OE2	1:F:700:VAL:HG13	2.18	0.44
1:A:685:MET:HG3	1:A:721:VAL:HG13	2.00	0.44
1:C:313:LYS:HE3	1:C:313:LYS:HB2	1.79	0.44
1:G:311:MET:HE1	1:G:476:MET:HG2	1.97	0.44
2:H:174:LYS:HE2	2:H:174:LYS:HB3	1.76	0.44
1:B:362:GLN:HE21	1:A:339:THR:HG21	1.83	0.44
1:B:657:GLN:HA	1:B:746:VAL:O	2.17	0.44
1:D:547:LYS:HG3	1:D:565:LEU:HD11	2.00	0.44
1:G:693:THR:OG1	1:G:744:THR:HG21	2.18	0.44
1:A:680:ASN:ND2	1:A:770:GLN:HG2	2.33	0.44
1:E:641:TYR:O	1:E:663:ALA:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:687:MET:HA	1:F:687:MET:HE2	1.98	0.44
2:H:301:GLY:O	2:H:306:ASP:HB3	2.18	0.44
1:B:681:TYR:HB3	1:B:753:ILE:CD1	2.48	0.43
1:C:442:LYS:HD3	1:C:442:LYS:HA	1.75	0.43
1:C:638:GLY:HA3	1:C:666:ALA:O	2.18	0.43
1:C:780:TYR:CG	1:C:780:TYR:O	2.70	0.43
1:F:640:TRP:HE3	1:F:643:THR:HG21	1.83	0.43
1:A:362:GLN:HE21	1:G:339:THR:HG21	1.83	0.43
1:C:375:LYS:HE3	1:C:375:LYS:HB2	1.77	0.43
1:F:311:MET:HE3	1:F:478:LEU:HG	2.00	0.43
1:F:687:MET:HB3	1:F:713:LEU:CD2	2.48	0.43
1:E:272:HIS:HD2	1:E:276:ASP:O	2.02	0.43
1:F:375:LYS:HE2	1:F:375:LYS:HB3	1.79	0.43
1:C:243:THR:HG23	1:C:252:TRP:CE3	2.52	0.43
1:E:641:TYR:HD2	1:E:664:TYR:CZ	2.36	0.43
1:F:635:LYS:HD2	1:F:638:GLY:O	2.18	0.43
1:G:665:VAL:O	1:G:735:LYS:HA	2.19	0.43
1:G:772:ILE:HG13	1:G:773:PHE:HD1	1.83	0.43
2:H:308:LYS:HE2	2:H:308:LYS:HB2	1.86	0.43
1:A:418:THR:H	1:G:392:ASN:ND2	2.14	0.43
1:A:662:ASN:O	1:A:664:TYR:HD1	2.02	0.43
1:C:661:SER:HA	1:C:740:GLY:H	1.84	0.43
1:A:410:THR:HB	1:A:478:LEU:HD22	2.01	0.43
1:A:628:ALA:HB2	1:A:656:PHE:CE2	2.54	0.43
1:F:697:VAL:HG22	1:F:738:ILE:HG12	2.00	0.43
1:G:780:TYR:O	1:G:780:TYR:CG	2.70	0.43
1:D:735:LYS:HE2	1:D:737:TYR:HE1	1.84	0.42
1:F:478:LEU:HD23	1:F:478:LEU:HA	1.88	0.42
1:F:628:ALA:HB2	1:F:656:PHE:CE2	2.54	0.42
1:C:657:GLN:HA	1:C:746:VAL:O	2.19	0.42
1:D:410:THR:HB	1:D:478:LEU:HD22	2.00	0.42
1:E:711:VAL:HG23	1:E:713:LEU:HD11	2.01	0.42
1:A:290:MET:HE3	1:A:290:MET:HB3	1.83	0.42
1:D:272:HIS:HD2	1:D:276:ASP:O	2.03	0.42
1:E:288:LEU:O	1:E:289:ASP:C	2.62	0.42
1:G:350:PRO:HG2	1:G:351:LYS:HD2	2.01	0.42
1:C:224:GLU:HG2	1:C:236:LEU:HD12	2.01	0.42
1:F:685:MET:CE	1:F:697:VAL:HG11	2.49	0.42
1:B:664:TYR:HB3	1:B:737:TYR:CE1	2.54	0.42
1:C:641:TYR:HB2	1:C:664:TYR:CE1	2.55	0.42
1:C:656:PHE:HB2	1:C:748:TRP:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:559:LYS:HZ3	1:C:569:ASP:H	1.67	0.42
1:C:699:VAL:HG23	1:C:706:ILE:HB	2.01	0.42
1:G:693:THR:HG22	1:G:694:GLU:N	2.35	0.42
1:C:392:ASN:HD21	1:D:418:THR:H	1.66	0.42
1:G:272:HIS:HD2	1:G:276:ASP:O	2.03	0.42
1:G:434:SER:HB2	1:G:437:GLU:HG3	2.02	0.42
1:A:559:LYS:NZ	1:A:559:LYS:HB3	2.34	0.42
1:A:683:LEU:O	1:A:722:ASP:HA	2.20	0.42
1:D:476:MET:HE3	1:D:476:MET:HB2	1.94	0.42
1:F:635:LYS:HE3	1:F:639:THR:HG23	2.02	0.42
1:G:570:LYS:HB3	1:G:570:LYS:HE2	1.73	0.42
1:G:705:THR:HG22	1:G:706:ILE:HG23	2.01	0.42
1:G:579:THR:HG21	1:G:606:LEU:HD21	2.01	0.42
1:E:392:ASN:ND2	1:F:418:THR:H	2.17	0.42
1:E:570:LYS:HB3	1:E:570:LYS:HE2	1.79	0.42
1:G:711:VAL:HG23	1:G:713:LEU:HB2	2.02	0.42
1:A:278:TYR:CD2	1:A:288:LEU:HD12	2.54	0.41
1:D:688:LYS:HB3	1:D:688:LYS:HE2	1.82	0.41
1:E:703:LYS:HE2	1:E:731:ASN:HD21	1.85	0.41
1:F:392:ASN:ND2	1:G:418:THR:H	2.18	0.41
1:F:730:ARG:HG2	1:F:773:PHE:CZ	2.55	0.41
1:B:416:LYS:HE3	1:B:416:LYS:HB2	1.81	0.41
1:C:470:LEU:HD21	1:C:476:MET:HE3	2.02	0.41
1:D:641:TYR:HD1	1:D:664:TYR:CZ	2.37	0.41
1:B:410:THR:HB	1:B:478:LEU:HD22	2.02	0.41
1:B:624:LEU:HB2	1:B:753:ILE:HG23	2.02	0.41
1:C:678:SER:O	1:C:776:SER:HB3	2.20	0.41
1:D:679:VAL:HG23	1:D:681:TYR:CE1	2.55	0.41
1:E:272:HIS:CE1	1:E:279:THR:HG22	2.56	0.41
1:F:272:HIS:HD2	1:F:276:ASP:O	2.03	0.41
1:F:332:THR:HG23	1:F:369:GLN:HG2	2.01	0.41
1:B:392:ASN:ND2	1:C:418:THR:H	2.19	0.41
1:B:700:VAL:HG22	1:B:704:SER:HA	2.01	0.41
1:C:700:VAL:HG13	1:C:735:LYS:HG3	2.02	0.41
1:G:272:HIS:CE1	1:G:279:THR:HG22	2.55	0.41
1:B:714:ASN:HD22	1:B:716:GLN:HE22	1.67	0.41
1:G:683:LEU:HB3	1:G:723:ILE:HD11	2.02	0.41
1:E:686:TYR:CE2	1:E:720:ARG:HB2	2.55	0.41
1:G:478:LEU:HD23	1:G:478:LEU:HA	1.87	0.41
1:B:684:SER:HA	1:B:721:VAL:O	2.21	0.41
1:B:243:THR:HG22	1:B:262:THR:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:587:LYS:HE3	1:B:587:LYS:HB2	1.66	0.41
1:A:643:THR:HA	1:A:658:SER:OG	2.21	0.41
1:B:272:HIS:HD2	1:B:276:ASP:O	2.04	0.41
1:C:478:LEU:HD23	1:C:478:LEU:HA	1.93	0.41
1:D:304:PHE:CE1	1:D:528:ARG:HG3	2.56	0.41
1:G:300:LEU:HD13	1:G:544:LEU:HD11	2.03	0.41
1:G:656:PHE:HB2	1:G:748:TRP:CE2	2.56	0.41
1:G:683:LEU:HB3	1:G:723:ILE:CD1	2.51	0.41
1:B:312:GLU:O	1:B:313:LYS:HG3	2.21	0.41
1:B:653:LYS:HE2	1:B:653:LYS:HB2	1.53	0.41
1:A:490:LYS:HB2	1:A:490:LYS:HE3	1.89	0.41
1:A:584:ASN:H	1:A:584:ASN:ND2	2.18	0.41
1:A:713:LEU:HD12	1:A:713:LEU:H	1.86	0.40
1:F:780:TYR:O	1:F:780:TYR:CG	2.74	0.40
1:G:659:ALA:HB2	1:G:745:ASN:HA	2.01	0.40
1:B:697:VAL:HG12	1:B:738:ILE:HG12	2.02	0.40
1:D:392:ASN:HD21	1:E:418:THR:H	1.68	0.40
1:F:287:ASP:OD2	1:F:490:LYS:HD2	2.20	0.40
1:F:442:LYS:HA	1:F:442:LYS:HE2	2.02	0.40
1:G:701:GLY:HA2	1:G:734:ASP:OD1	2.21	0.40
1:B:678:SER:HA	1:B:726:LYS:HE3	2.02	0.40
1:A:564:LEU:HB3	1:A:573:TYR:CD2	2.56	0.40
1:C:410:THR:HB	1:C:478:LEU:HD22	2.04	0.40
1:D:728:SER:HB2	1:D:773:PHE:CE1	2.55	0.40
1:F:675:LEU:HG	1:F:681:TYR:CZ	2.56	0.40
1:G:416:LYS:HE3	1:G:416:LYS:HB2	1.76	0.40
1:A:276:ASP:HB2	1:A:277:PRO:CD	2.51	0.40
1:F:735:LYS:HE3	1:F:737:TYR:CE1	2.50	0.40
1:C:587:LYS:HB3	1:C:587:LYS:HE2	1.84	0.40
1:C:677:GLN:NE2	1:C:729:GLU:HG2	2.37	0.40
1:D:728:SER:HB2	1:D:773:PHE:CZ	2.57	0.40
1:E:490:LYS:HE3	1:E:490:LYS:HB2	1.87	0.40
1:E:684:SER:HB2	1:E:752:THR:OG1	2.21	0.40
1:G:714:ASN:HD21	1:G:716:GLN:HG2	1.87	0.40
2:H:304:ARG:NE	2:H:423:PHE:CD2	2.90	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	558/656 (85%)	537 (96%)	21 (4%)	0	100	100
1	B	558/656 (85%)	542 (97%)	16 (3%)	0	100	100
1	C	558/656 (85%)	539 (97%)	19 (3%)	0	100	100
1	D	558/656 (85%)	546 (98%)	12 (2%)	0	100	100
1	E	558/656 (85%)	542 (97%)	16 (3%)	0	100	100
1	F	558/656 (85%)	542 (97%)	16 (3%)	0	100	100
1	G	558/656 (85%)	543 (97%)	15 (3%)	0	100	100
2	H	387/390 (99%)	381 (98%)	6 (2%)	0	100	100
All	All	4293/4982 (86%)	4172 (97%)	121 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	489/573 (85%)	489 (100%)	0	100	100
1	B	489/573 (85%)	489 (100%)	0	100	100
1	C	489/573 (85%)	489 (100%)	0	100	100
1	D	489/573 (85%)	489 (100%)	0	100	100
1	E	489/573 (85%)	489 (100%)	0	100	100
1	F	489/573 (85%)	489 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	489/573 (85%)	489 (100%)	0	100	100
2	H	341/342 (100%)	341 (100%)	0	100	100
All	All	3764/4353 (86%)	3764 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (99) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	246	ASN
1	B	272	HIS
1	B	333	ASN
1	B	382	ASN
1	B	392	ASN
1	B	473	ASN
1	B	481	ASN
1	B	507	GLN
1	B	568	ASN
1	B	604	ASN
1	B	616	ASN
1	B	642	ASN
1	B	660	ASN
1	B	677	GLN
1	B	716	GLN
1	B	731	ASN
1	A	272	HIS
1	A	308	ASN
1	A	362	GLN
1	A	382	ASN
1	A	392	ASN
1	A	456	ASN
1	A	568	ASN
1	A	584	ASN
1	A	642	ASN
1	A	662	ASN
1	A	715	ASN
1	C	246	ASN
1	C	272	HIS
1	C	324	ASN
1	C	392	ASN
1	C	432	ASN

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Mol	Chain	Res	Type
1	C	458	HIS
1	C	473	ASN
1	C	481	ASN
1	C	568	ASN
1	C	616	ASN
1	C	660	ASN
1	C	677	GLN
1	C	715	ASN
1	C	779	GLN
1	D	246	ASN
1	D	272	HIS
1	D	369	GLN
1	D	382	ASN
1	D	392	ASN
1	D	432	ASN
1	D	444	GLN
1	D	469	GLN
1	D	481	ASN
1	D	568	ASN
1	D	716	GLN
1	E	246	ASN
1	E	272	HIS
1	E	392	ASN
1	E	432	ASN
1	E	473	ASN
1	E	568	ASN
1	E	584	ASN
1	E	616	ASN
1	E	660	ASN
1	E	676	ASN
1	E	680	ASN
1	E	719	GLN
1	E	731	ASN
1	F	246	ASN
1	F	272	HIS
1	F	321	ASN
1	F	329	HIS
1	F	392	ASN
1	F	432	ASN
1	F	473	ASN
1	F	568	ASN
1	F	616	ASN

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Mol	Chain	Res	Type
1	F	647	ASN
1	F	745	ASN
1	G	246	ASN
1	G	272	HIS
1	G	308	ASN
1	G	321	ASN
1	G	329	HIS
1	G	362	GLN
1	G	382	ASN
1	G	392	ASN
1	G	432	ASN
1	G	456	ASN
1	G	495	ASN
1	G	568	ASN
1	G	616	ASN
1	G	647	ASN
1	G	677	GLN
1	G	680	ASN
1	G	714	ASN
1	G	731	ASN
2	H	107	ASN
2	H	228	ASN
2	H	236	ASN
2	H	283	ASN
2	H	407	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 21 ligands modelled in this entry, 21 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.