



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Sep 27, 2017 – 05:15 AM EDT

PDB ID : 5NER
EMDB ID: : EMD-3633
Title : Localised reconstruction of alpha v beta 6 bound to Foot and Mouth Disease
Virus O PanAsia - Pose A prime.
Authors : Kotecha, A.; Stuart, D.
Deposited on : unknown
Resolution : 11.50 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
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

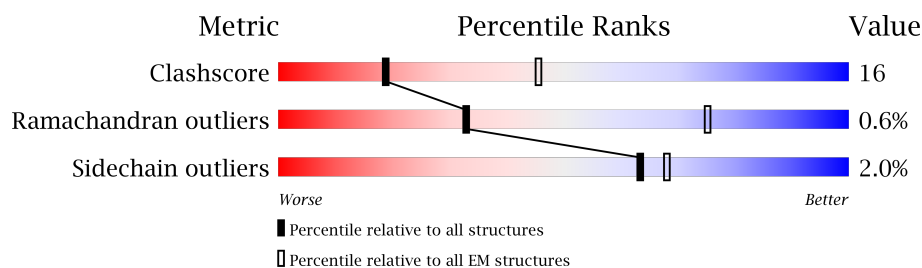
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 11.50 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	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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	1	210	
2	2	214	
3	3	220	
4	4	70	
5	A	594	
6	B	470	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	MAN	A	606	X	-	-	-
7	MAN	A	610	X	-	-	-
7	MAN	A	614	-	-	X	-
8	NAG	A	607	-	-	X	-
8	NAG	A	612	-	-	X	-
8	NAG	A	613	-	-	X	-
8	NAG	B	501	X	-	-	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 13639 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 O PanAsia VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	210	Total	C	N	O	S	0	0
			1638	1033	295	306	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	155	VAL	ALA	conflict	UNP A0A1P8NWT0

- Molecule 2 is a protein called O PanAsia VP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	214	Total	C	N	O	S	0	0
			1677	1065	286	319	7		

- Molecule 3 is a protein called O PanAsia VP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	220	Total	C	N	O	S	0	0
			1686	1080	275	322	9		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	56	ARG	HIS	engineered mutation	UNP J3T9N5

- Molecule 4 is a protein called O PanAsia VP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	47	Total	C	N	O	S	0	1
			354	222	58	72	2		

- Molecule 5 is a protein called Integrin alpha-V.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	589	Total	C	N	O	S	0	0
			4564	2894	774	875	21		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	400	CYS	MET	conflict	UNP P06756

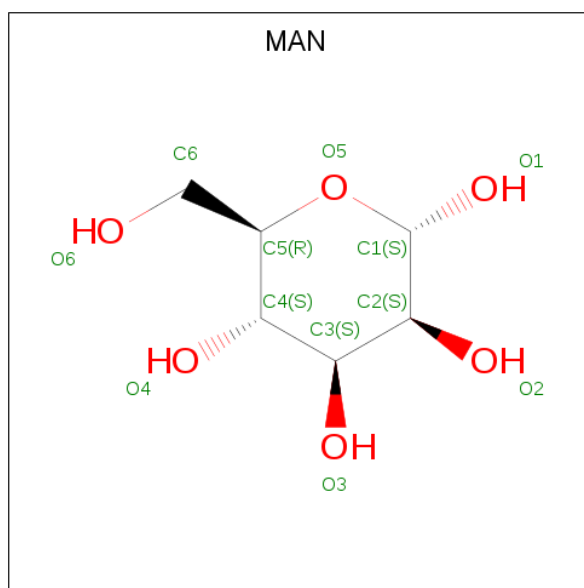
- Molecule 6 is a protein called Integrin beta-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	448	Total	C	N	O	S	0	0
			3438	2157	587	663	31		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	267	CYS	ILE	conflict	UNP P18564
B	449	ASN	HIS	conflict	UNP P18564

- Molecule 7 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C₆H₁₂O₆).



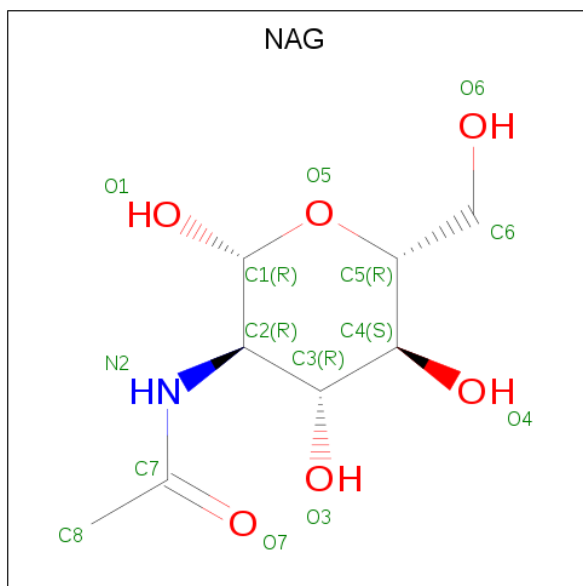
Mol	Chain	Residues	Atoms			AltConf
7	1	1	Total	C	O	0
			22	12	10	
7	1	1	Total	C	O	0
			22	12	10	

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Mol	Chain	Residues	Atoms			AltConf
7	2	1	Total	C	O	0
			22	12	10	
7	2	1	Total	C	O	0
			22	12	10	
7	3	1	Total	C	O	0
			11	6	5	
7	A	1	Total	C	O	0
			69	36	33	
7	A	1	Total	C	O	0
			69	36	33	
7	A	1	Total	C	O	0
			69	36	33	
7	A	1	Total	C	O	0
			69	36	33	
7	A	1	Total	C	O	0
			69	36	33	

- Molecule 8 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
8	A	1	Total	C	N	O	0
			126	72	9	45	
8	A	1	Total	C	N	O	0
			126	72	9	45	

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Mol	Chain	Residues	Atoms				AltConf
8	A	1	Total	C	N	O	0
			126	72	9	45	
8	A	1	Total	C	N	O	0
			126	72	9	45	
8	A	1	Total	C	N	O	0
			126	72	9	45	
8	A	1	Total	C	N	O	0
			126	72	9	45	
8	A	1	Total	C	N	O	0
			126	72	9	45	
8	A	1	Total	C	N	O	0
			126	72	9	45	
8	B	1	Total	C	N	O	0
			28	16	2	10	
8	B	1	Total	C	N	O	0
			28	16	2	10	

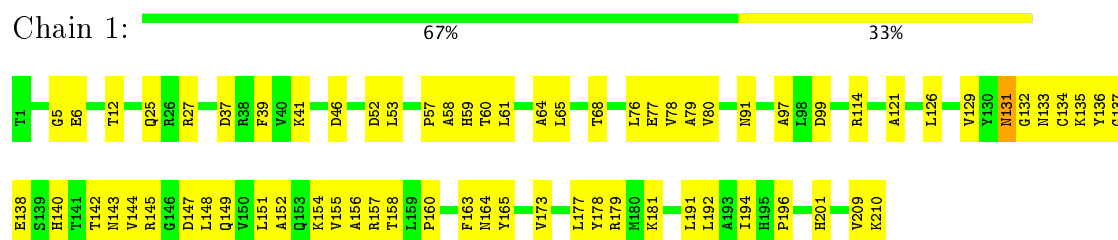
- Molecule 9 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
9	A	4	Total	Ca	0
			4	4	

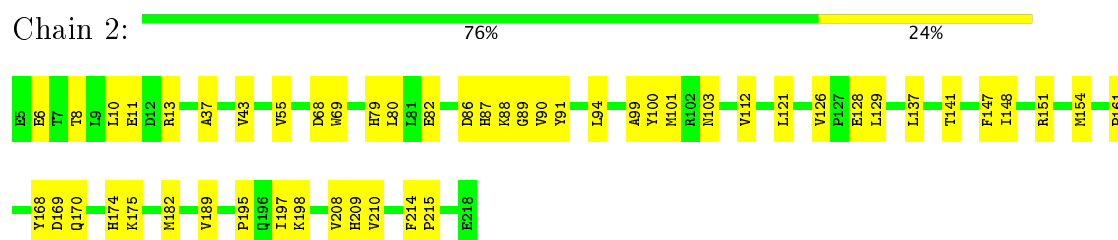
3 Residue-property plots

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.

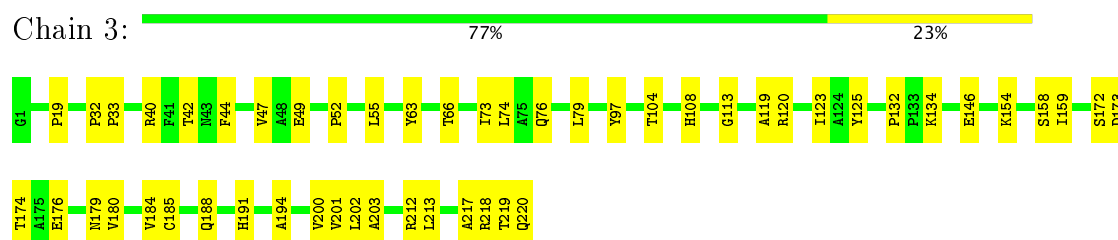
• Molecule 1: O PanAsia VP1



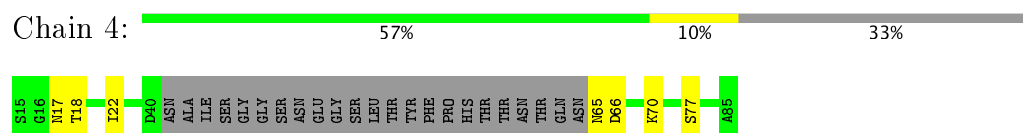
• Molecule 2: O PanAsia VP2



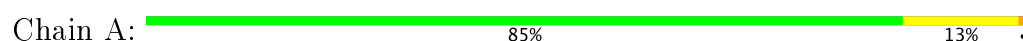
• Molecule 3: O PanAsia VP3

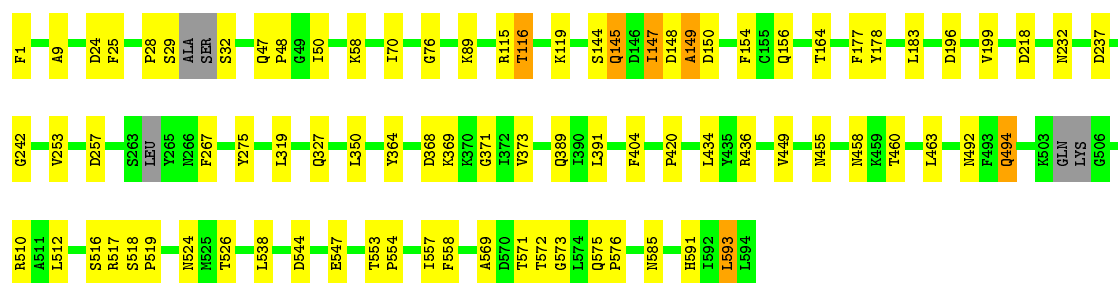


• Molecule 4: O PanAsia VP4



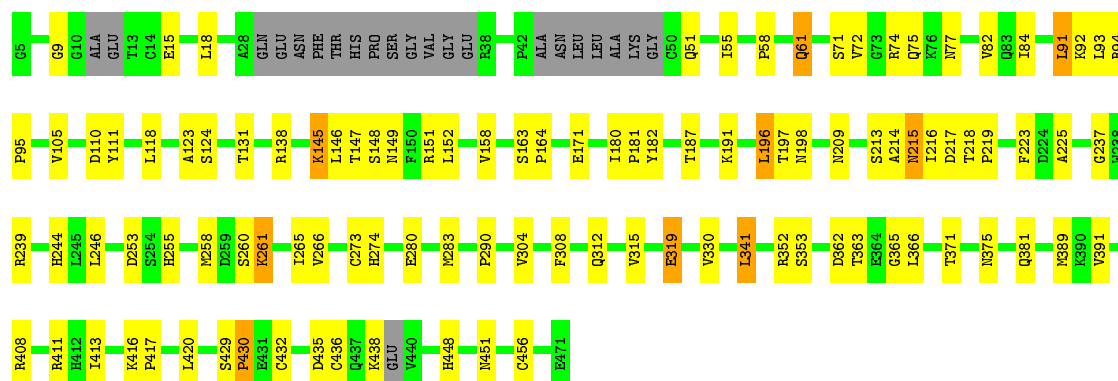
• Molecule 5: Integrin alpha-V





• Molecule 6: Integrin beta-6

Chain B: 73% 20% 5%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	13483	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	18	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	37037	Depositor
Image detector	GATAN K2 SUMMIT (4k 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, NAG, MAN

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	1	0.48	0/1675	0.60	0/2289
2	2	0.53	0/1720	0.55	0/2348
3	3	0.53	0/1735	0.56	0/2370
4	4	0.42	0/360	0.58	0/483
5	A	0.23	0/4665	0.40	0/6312
6	B	0.22	0/3497	0.40	0/4729
All	All	0.37	0/13652	0.48	0/18531

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	1	1638	0	1651	217	0
2	2	1677	0	1625	105	0
3	3	1686	0	1617	54	0
4	4	354	0	324	7	0
5	A	4564	0	4410	114	0
6	B	3438	0	3378	98	0
7	1	22	0	20	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	2	22	0	19	0	0
7	3	11	0	10	0	0
7	A	69	0	60	7	0
8	A	126	0	110	36	0
8	B	28	0	26	0	0
9	A	4	0	0	0	0
All	All	13639	0	13250	433	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 16.

All (433) 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)
2:2:99:ALA:HB2	2:2:214:PHE:CZ	1.27	1.61
1:1:134:CYS:SG	1:1:156:ALA:HB1	1.44	1.53
1:1:135:LYS:CD	2:2:80:LEU:HD23	1.08	1.52
1:1:135:LYS:HD3	2:2:80:LEU:CD2	1.01	1.46
5:A:585:ASN:ND2	8:A:612:NAG:C1	1.79	1.45
2:2:99:ALA:CB	2:2:214:PHE:CZ	1.97	1.42
5:A:585:ASN:CG	8:A:612:NAG:C1	1.87	1.40
1:1:142:THR:OG1	5:A:150:ASP:HB2	1.21	1.37
5:A:585:ASN:OD1	8:A:612:NAG:C1	1.69	1.36
1:1:145:ARG:N	5:A:178:TYR:CZ	1.81	1.34
1:1:138:GLU:OE1	2:2:79:HIS:ND1	1.59	1.34
1:1:135:LYS:NZ	2:2:80:LEU:HD21	1.37	1.34
1:1:151:LEU:HD22	6:B:123:ALA:CB	1.58	1.33
1:1:155:VAL:HG22	6:B:180:ILE:CD1	1.60	1.28
1:1:135:LYS:CD	2:2:80:LEU:CD2	1.76	1.28
1:1:142:THR:C	5:A:150:ASP:HB3	1.53	1.26
5:A:558:PHE:HE1	8:A:612:NAG:C8	1.47	1.26
2:2:99:ALA:HB2	2:2:214:PHE:CE1	1.71	1.25
1:1:135:LYS:N	2:2:82:GLU:OE2	1.70	1.23
6:B:110:ASP:CG	6:B:148:SER:HA	1.55	1.20
6:B:74:ARG:NH1	6:B:145:LYS:HA	1.57	1.19
1:1:135:LYS:HD2	2:2:80:LEU:HD23	1.26	1.18
5:A:585:ASN:HD21	8:A:612:NAG:C1	1.46	1.18
1:1:135:LYS:CE	2:2:80:LEU:CD2	2.24	1.15
1:1:145:ARG:HB3	5:A:178:TYR:CG	1.80	1.15
1:1:145:ARG:HB3	5:A:178:TYR:CD2	1.80	1.15
1:1:155:VAL:HG22	6:B:180:ILE:HD12	1.17	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:142:THR:O	5:A:178:TYR:HE2	1.29	1.13
1:1:142:THR:O	5:A:150:ASP:HB3	1.46	1.13
1:1:143:ASN:ND2	5:A:148:ASP:OD2	1.80	1.12
1:1:151:LEU:CD2	6:B:123:ALA:HB1	1.79	1.12
1:1:135:LYS:HD3	2:2:80:LEU:HD22	1.17	1.10
1:1:135:LYS:CE	2:2:80:LEU:HD21	1.81	1.10
8:A:612:NAG:H62	8:A:613:NAG:H82	1.33	1.10
1:1:134:CYS:SG	1:1:156:ALA:CB	2.38	1.10
6:B:74:ARG:CZ	6:B:145:LYS:HA	1.72	1.10
1:1:151:LEU:HB2	6:B:123:ALA:O	1.52	1.08
6:B:110:ASP:CG	6:B:148:SER:CA	2.14	1.07
1:1:142:THR:C	5:A:150:ASP:CB	2.21	1.07
1:1:135:LYS:NZ	2:2:129:LEU:CD2	2.18	1.07
2:2:99:ALA:CB	2:2:214:PHE:HZ	1.50	1.07
5:A:558:PHE:HE1	8:A:612:NAG:H81	1.09	1.06
5:A:558:PHE:CE1	8:A:612:NAG:C8	2.39	1.05
1:1:143:ASN:OD1	5:A:148:ASP:O	1.74	1.05
5:A:558:PHE:CE1	8:A:612:NAG:H81	1.91	1.05
1:1:135:LYS:NZ	2:2:129:LEU:HD21	1.72	1.05
1:1:142:THR:O	5:A:178:TYR:CE2	2.11	1.03
6:B:74:ARG:NH1	6:B:145:LYS:CA	2.21	1.02
6:B:74:ARG:CZ	6:B:145:LYS:CA	2.34	1.02
6:B:110:ASP:OD2	6:B:148:SER:HA	1.57	1.02
1:1:132:GLY:O	2:2:175:LYS:N	1.92	1.02
1:1:145:ARG:CD	5:A:218:ASP:OD2	2.08	1.01
1:1:137:GLY:H	2:2:80:LEU:CB	1.73	1.01
3:3:42:THR:HG1	4:4:65:ASN:N	1.58	1.00
1:1:135:LYS:NZ	2:2:80:LEU:CD2	2.21	0.99
1:1:142:THR:OG1	5:A:150:ASP:CB	2.10	0.99
1:1:145:ARG:HE	5:A:178:TYR:HB2	1.28	0.98
5:A:524:ASN:HD21	8:A:611:NAG:C1	1.75	0.98
1:1:135:LYS:HZ2	2:2:129:LEU:CD2	1.75	0.98
1:1:135:LYS:HE3	2:2:129:LEU:HG	1.47	0.97
1:1:145:ARG:CB	5:A:178:TYR:CE2	2.49	0.96
1:1:77:GLU:OE1	1:1:181:LYS:NZ	1.99	0.95
1:1:145:ARG:HE	5:A:178:TYR:CB	1.79	0.94
1:1:145:ARG:NE	5:A:218:ASP:OD2	2.00	0.94
1:1:145:ARG:N	5:A:178:TYR:CE1	2.35	0.94
1:1:145:ARG:NH2	5:A:177:PHE:C	2.22	0.93
1:1:145:ARG:HB3	5:A:178:TYR:CD1	2.04	0.92
1:1:194:ILE:HD11	3:3:219:THR:OG1	1.69	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:135:LYS:HZ3	2:2:80:LEU:HD21	1.20	0.92
1:1:145:ARG:NH2	5:A:177:PHE:O	2.02	0.92
1:1:136:TYR:O	2:2:80:LEU:O	1.88	0.91
1:1:145:ARG:HD2	5:A:218:ASP:OD2	1.70	0.91
1:1:145:ARG:CB	5:A:178:TYR:CD2	2.52	0.91
6:B:74:ARG:HH12	6:B:145:LYS:N	1.58	0.90
1:1:151:LEU:HD22	6:B:123:ALA:HB1	0.91	0.90
1:1:145:ARG:HB3	5:A:178:TYR:CE2	2.07	0.90
1:1:145:ARG:HH21	5:A:178:TYR:HB2	1.34	0.89
1:1:145:ARG:HH21	5:A:177:PHE:C	1.75	0.89
1:1:137:GLY:H	2:2:80:LEU:HB2	1.36	0.89
1:1:142:THR:HG1	5:A:150:ASP:HB2	1.06	0.89
1:1:129:VAL:HG11	2:2:128:GLU:O	1.72	0.88
1:1:77:GLU:OE2	1:1:114:ARG:NH2	2.06	0.87
1:1:145:ARG:NE	5:A:178:TYR:HB2	1.88	0.87
2:2:99:ALA:CA	2:2:214:PHE:CZ	2.58	0.86
1:1:155:VAL:CG2	6:B:180:ILE:HD12	2.04	0.86
2:2:99:ALA:HB1	2:2:214:PHE:HZ	1.37	0.86
1:1:132:GLY:O	2:2:174:HIS:HA	1.74	0.86
1:1:145:ARG:NH2	5:A:178:TYR:HB2	1.91	0.86
1:1:135:LYS:HZ1	2:2:129:LEU:HD21	1.40	0.86
5:A:585:ASN:ND2	8:A:612:NAG:O5	2.08	0.85
1:1:135:LYS:CE	2:2:129:LEU:HG	2.06	0.85
1:1:137:GLY:N	2:2:80:LEU:HB2	1.90	0.85
1:1:155:VAL:CG2	6:B:180:ILE:CD1	2.53	0.84
1:1:135:LYS:HZ2	2:2:80:LEU:HD21	1.41	0.84
1:1:145:ARG:CA	5:A:178:TYR:CZ	2.60	0.84
5:A:524:ASN:ND2	8:A:611:NAG:C1	2.41	0.83
6:B:74:ARG:NH1	6:B:145:LYS:N	2.18	0.83
1:1:137:GLY:CA	2:2:80:LEU:HB2	2.07	0.83
1:1:126:LEU:HD22	1:1:163:PHE:HB3	1.60	0.82
1:1:148:LEU:CD2	6:B:215:ASN:O	2.28	0.82
1:1:143:ASN:N	5:A:150:ASP:CB	2.40	0.82
1:1:91:ASN:CG	1:1:164:ASN:O	2.18	0.81
1:1:148:LEU:HG	6:B:215:ASN:O	1.81	0.80
1:1:135:LYS:HZ1	2:2:129:LEU:CD2	1.91	0.79
1:1:145:ARG:HB2	5:A:178:TYR:CE2	2.17	0.79
1:1:138:GLU:OE1	2:2:79:HIS:CG	2.36	0.79
6:B:74:ARG:NH2	6:B:146:LEU:N	2.30	0.79
1:1:148:LEU:CD1	6:B:216:ILE:HA	2.13	0.79
1:1:64:ALA:O	1:1:68:THR:HG23	1.82	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:111:TYR:HD1	6:B:352:ARG:HB2	1.48	0.78
1:1:145:ARG:CB	5:A:178:TYR:CZ	2.67	0.78
6:B:110:ASP:OD1	6:B:148:SER:N	2.18	0.77
1:1:145:ARG:O	5:A:178:TYR:CE1	2.37	0.77
1:1:132:GLY:HA2	2:2:174:HIS:HA	1.67	0.77
1:1:132:GLY:O	2:2:174:HIS:CA	2.33	0.77
1:1:134:CYS:CB	1:1:156:ALA:HB1	2.15	0.76
8:A:613:NAG:C3	7:A:614:MAN:H2	2.15	0.76
1:1:59:HIS:HA	3:3:220:GLN:HB2	1.65	0.76
1:1:145:ARG:CA	5:A:178:TYR:CE1	2.69	0.76
1:1:155:VAL:HG22	6:B:180:ILE:HD11	1.62	0.76
3:3:173:ASP:H	3:3:179:ASN:HD22	1.34	0.75
1:1:91:ASN:ND2	1:1:164:ASN:O	2.20	0.75
8:A:612:NAG:O3	8:A:613:NAG:O5	2.03	0.75
1:1:145:ARG:CZ	5:A:178:TYR:HB2	2.17	0.74
1:1:135:LYS:HZ1	2:2:129:LEU:CG	2.00	0.74
1:1:135:LYS:HZ2	2:2:129:LEU:HD23	1.51	0.74
2:2:99:ALA:HA	2:2:214:PHE:CE2	2.23	0.74
1:1:194:ILE:CD1	3:3:219:THR:OG1	2.36	0.73
8:A:607:NAG:H61	8:A:608:NAG:O7	1.89	0.73
1:1:58:ALA:O	3:3:220:GLN:HB2	1.89	0.73
6:B:110:ASP:OD1	6:B:148:SER:CA	2.36	0.73
6:B:147:THR:HG22	6:B:149:ASN:H	1.54	0.73
1:1:27:ARG:NH2	3:3:49:GLU:OE2	2.18	0.72
1:1:129:VAL:CG1	2:2:128:GLU:O	2.37	0.72
5:A:460:THR:HB	8:A:607:NAG:H62	1.71	0.72
5:A:558:PHE:HE1	8:A:612:NAG:H82	1.51	0.72
2:2:11:GLU:OE2	2:2:13:ARG:NH2	2.22	0.72
1:1:132:GLY:C	2:2:174:HIS:HA	2.09	0.72
1:1:58:ALA:HB1	3:3:220:GLN:OE1	1.89	0.72
1:1:137:GLY:N	2:2:80:LEU:CB	2.50	0.72
1:1:132:GLY:CA	2:2:174:HIS:HA	2.19	0.72
1:1:143:ASN:OD1	5:A:148:ASP:CB	2.38	0.71
1:1:148:LEU:CG	6:B:215:ASN:O	2.38	0.71
1:1:135:LYS:NZ	2:2:129:LEU:CG	2.53	0.71
8:A:612:NAG:H62	8:A:613:NAG:C8	2.17	0.71
6:B:74:ARG:NH2	6:B:145:LYS:C	2.43	0.71
3:3:174:THR:O	3:3:179:ASN:ND2	2.20	0.70
8:A:613:NAG:H3	7:A:614:MAN:H2	1.72	0.70
1:1:133:ASN:OD1	2:2:175:LYS:HG2	1.92	0.70
1:1:148:LEU:HG	6:B:216:ILE:HA	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:145:ARG:HB3	5:A:178:TYR:CE1	2.27	0.69
1:1:142:THR:CB	5:A:150:ASP:HB2	2.22	0.69
1:1:135:LYS:HZ2	2:2:80:LEU:CD2	1.99	0.69
2:2:86:ASP:OD2	2:2:88:LYS:NZ	2.25	0.69
1:1:151:LEU:CD2	6:B:123:ALA:CB	2.52	0.68
1:1:148:LEU:HD21	6:B:215:ASN:O	1.93	0.68
1:1:145:ARG:HB3	5:A:178:TYR:CZ	2.28	0.68
1:1:143:ASN:OD1	5:A:148:ASP:HB3	1.94	0.68
1:1:137:GLY:H	2:2:80:LEU:HB3	1.56	0.68
1:1:192:LEU:O	3:3:220:GLN:O	2.12	0.67
5:A:232:ASN:ND2	5:A:257:ASP:OD2	2.28	0.67
1:1:135:LYS:NZ	2:2:129:LEU:HG	2.09	0.67
1:1:137:GLY:HA3	2:2:80:LEU:HB2	1.77	0.66
1:1:57:PRO:HB2	1:1:60:THR:HG23	1.78	0.66
1:1:147:ASP:N	6:B:218:THR:HA	2.10	0.66
1:1:52:ASP:OD2	1:1:160:PRO:HB2	1.95	0.66
5:A:585:ASN:OD1	8:A:612:NAG:C2	2.44	0.65
2:2:55:VAL:HG11	2:2:94:LEU:HD21	1.78	0.65
2:2:101:MET:HG2	2:2:210:VAL:HG12	1.79	0.65
8:A:607:NAG:H61	8:A:608:NAG:C7	2.26	0.65
1:1:152:ALA:O	1:1:155:VAL:HG23	1.97	0.65
5:A:585:ASN:OD1	8:A:612:NAG:N2	2.29	0.65
1:1:145:ARG:C	5:A:178:TYR:CE1	2.71	0.65
1:1:132:GLY:O	2:2:174:HIS:C	2.35	0.65
6:B:417:PRO:HG2	6:B:420:LEU:HB2	1.77	0.65
2:2:99:ALA:CA	2:2:214:PHE:CE2	2.79	0.64
7:A:614:MAN:H3	7:A:615:MAN:O1	1.98	0.64
1:1:145:ARG:HH21	5:A:178:TYR:CB	2.09	0.64
6:B:158:VAL:HG21	6:B:213:SER:HB2	1.80	0.64
1:1:131:ASN:HD22	2:2:129:LEU:N	1.96	0.63
1:1:143:ASN:OD1	5:A:148:ASP:CG	2.37	0.63
3:3:66:THR:OG1	3:3:194:ALA:O	2.12	0.63
1:1:64:ALA:CB	3:3:220:GLN:HG3	2.28	0.63
6:B:363:THR:HB	6:B:366:LEU:HB2	1.79	0.63
3:3:108:HIS:HB2	3:3:202:LEU:HB2	1.81	0.63
1:1:148:LEU:CG	6:B:216:ILE:HA	2.28	0.63
1:1:136:TYR:N	1:1:137:GLY:HA2	2.13	0.63
1:1:77:GLU:HB3	1:1:179:ARG:HB3	1.81	0.62
1:1:147:ASP:HB2	6:B:218:THR:HA	1.82	0.62
1:1:64:ALA:HB1	3:3:220:GLN:HG3	1.82	0.61
3:3:52:PRO:HB2	3:3:202:LEU:HB3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:135:LYS:O	2:2:82:GLU:CD	2.39	0.61
2:2:141:THR:OG1	3:3:52:PRO:O	2.14	0.61
5:A:558:PHE:CE1	8:A:612:NAG:H82	2.29	0.61
8:A:613:NAG:H5	7:A:614:MAN:O1	2.00	0.61
1:1:25:GLN:OE1	1:1:25:GLN:N	2.34	0.60
3:3:176:GLU:O	3:3:180:VAL:HG12	2.01	0.60
1:1:132:GLY:HA3	1:1:157:ARG:HG3	1.83	0.60
1:1:6:GLU:HB3	2:2:147:PHE:HB2	1.82	0.60
8:A:612:NAG:C6	8:A:613:NAG:H82	2.21	0.60
5:A:9:ALA:HB3	5:A:434:LEU:HB3	1.84	0.60
1:1:135:LYS:HZ2	2:2:129:LEU:HD21	1.45	0.60
2:2:214:PHE:HB3	2:2:215:PRO:HD2	1.82	0.60
1:1:78:VAL:O	1:1:114:ARG:HA	2.02	0.59
1:1:137:GLY:HA3	2:2:80:LEU:HD22	1.83	0.59
2:2:69:TRP:HB3	2:2:197:ILE:HG23	1.83	0.59
3:3:76:GLN:HE21	3:3:132:PRO:HB2	1.68	0.59
1:1:147:ASP:CB	6:B:218:THR:HA	2.32	0.59
1:1:135:LYS:CA	2:2:82:GLU:OE2	2.50	0.59
5:A:58:LYS:HB2	5:A:70:ILE:HD11	1.83	0.59
1:1:133:ASN:CG	2:2:175:LYS:HZ2	2.06	0.59
1:1:209:VAL:HG12	1:1:210:LYS:HG2	1.84	0.59
8:A:602:NAG:H3	7:A:603:MAN:O1	2.02	0.59
6:B:371:THR:HG22	6:B:381:GLN:HA	1.83	0.59
1:1:143:ASN:O	5:A:149:ALA:HB3	2.03	0.58
6:B:362:ASP:O	6:B:411:ARG:NH1	2.36	0.58
1:1:58:ALA:O	3:3:220:GLN:OE1	2.21	0.58
1:1:138:GLU:OE1	2:2:79:HIS:HA	2.03	0.58
5:A:544:ASP:HB3	5:A:547:GLU:HG3	1.86	0.58
6:B:111:TYR:HA	6:B:352:ARG:HG3	1.86	0.58
5:A:492:ASN:HA	5:A:526:THR:HA	1.85	0.58
1:1:194:ILE:CG1	3:3:219:THR:OG1	2.52	0.58
1:1:145:ARG:HH21	5:A:178:TYR:N	2.02	0.58
1:1:134:CYS:SG	1:1:157:ARG:N	2.77	0.57
1:1:37:ASP:HB3	4:4:17:ASN:HB2	1.85	0.57
1:1:143:ASN:CG	5:A:148:ASP:OD2	2.41	0.57
5:A:460:THR:CB	8:A:607:NAG:H62	2.34	0.57
1:1:78:VAL:HG12	1:1:80:VAL:HG23	1.85	0.57
2:2:99:ALA:HA	2:2:214:PHE:CZ	2.35	0.57
1:1:145:ARG:NE	5:A:178:TYR:CD2	2.72	0.56
8:A:613:NAG:O3	7:A:614:MAN:H2	2.03	0.56
1:1:148:LEU:HD11	6:B:216:ILE:HA	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:91:TYR:OH	2:2:103:ASN:ND2	2.38	0.56
6:B:91:LEU:HD22	6:B:93:LEU:HG	1.87	0.56
1:1:65:LEU:HD12	3:3:44:PHE:CZ	2.42	0.55
5:A:24:ASP:OD1	5:A:25:PHE:N	2.37	0.55
6:B:260:SER:HB2	6:B:265:ILE:HB	1.89	0.55
5:A:510:ARG:NH1	5:A:553:THR:O	2.36	0.55
6:B:84:ILE:HD12	6:B:417:PRO:HD3	1.87	0.55
1:1:148:LEU:HD12	6:B:216:ILE:HG23	1.88	0.55
1:1:145:ARG:CB	5:A:178:TYR:CE1	2.89	0.55
2:2:126:VAL:HG11	2:2:129:LEU:HD13	1.88	0.54
5:A:50:ILE:HD13	5:A:89:LYS:HB2	1.88	0.54
6:B:74:ARG:HH12	6:B:145:LYS:CA	2.01	0.54
2:2:68:ASP:OD1	2:2:198:LYS:HG2	2.07	0.54
5:A:558:PHE:CE1	8:A:612:NAG:C7	2.89	0.54
6:B:274:HIS:CD2	6:B:283:MET:HG3	2.43	0.54
1:1:145:ARG:HA	1:1:149:GLN:HB2	1.89	0.54
5:A:319:LEU:HB2	5:A:327:GLN:HB3	1.90	0.54
2:2:37:ALA:HB3	2:2:161:PRO:HG3	1.88	0.54
6:B:187:THR:OG1	6:B:214:ALA:O	2.23	0.54
1:1:151:LEU:CG	6:B:123:ALA:HB1	2.38	0.54
1:1:135:LYS:HZ1	2:2:129:LEU:HG	1.70	0.54
1:1:147:ASP:N	6:B:218:THR:CA	2.70	0.54
5:A:115:ARG:NH1	5:A:116:THR:O	2.40	0.54
1:1:155:VAL:CG2	6:B:180:ILE:HD11	2.32	0.54
1:1:143:ASN:OD1	5:A:148:ASP:C	2.45	0.53
3:3:79:LEU:HD22	3:3:125:TYR:HE1	1.74	0.53
1:1:145:ARG:O	5:A:178:TYR:HE1	1.88	0.53
6:B:18:LEU:HA	6:B:94:ARG:HH21	1.74	0.53
2:2:103:ASN:HB3	2:2:208:VAL:HG12	1.90	0.53
1:1:133:ASN:CG	2:2:175:LYS:NZ	2.62	0.52
1:1:91:ASN:HD22	1:1:121:ALA:HA	1.75	0.52
1:1:68:THR:HG21	1:1:191:LEU:HD22	1.91	0.52
1:1:79:ALA:HB3	1:1:177:LEU:HB2	1.92	0.52
1:1:196:PRO:HB3	1:1:201:HIS:HB2	1.92	0.52
1:1:53:LEU:HD11	1:1:76:LEU:HD13	1.92	0.52
6:B:151:ARG:NH2	6:B:237:GLY:O	2.43	0.51
6:B:61:GLN:HB3	6:B:92:LYS:HE2	1.92	0.51
5:A:144:SER:OG	5:A:145:GLN:N	2.42	0.51
1:1:65:LEU:HD12	3:3:44:PHE:CE1	2.46	0.51
6:B:219:PRO:HB3	6:B:253:ASP:HB2	1.93	0.51
1:1:145:ARG:HH22	5:A:177:PHE:C	2.13	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:128:GLU:OE1	2:2:174:HIS:HE1	1.94	0.50
3:3:218:ARG:HG2	3:3:219:THR:N	2.27	0.50
5:A:29:SER:O	5:A:32:SER:N	2.45	0.50
5:A:585:ASN:OD1	8:A:612:NAG:C7	2.58	0.50
2:2:10:LEU:HD23	2:2:10:LEU:H	1.77	0.50
2:2:151:ARG:HD2	3:3:113:GLY:O	2.11	0.49
1:1:147:ASP:H	6:B:218:THR:CA	2.25	0.49
1:1:61:LEU:HD12	1:1:65:LEU:HD23	1.93	0.49
1:1:12:THR:O	4:4:77:SER:HA	2.12	0.49
1:1:151:LEU:CB	6:B:123:ALA:O	2.43	0.49
1:1:147:ASP:H	6:B:218:THR:HA	1.76	0.49
5:A:148:ASP:O	5:A:150:ASP:N	2.46	0.49
6:B:191:LYS:HG2	6:B:280:GLU:HG2	1.93	0.49
6:B:273:CYS:O	6:B:274:HIS:ND1	2.46	0.49
1:1:6:GLU:CB	2:2:147:PHE:HB2	2.42	0.49
2:2:99:ALA:CB	2:2:214:PHE:CE1	2.63	0.48
1:1:135:LYS:HD3	2:2:80:LEU:HD23	0.64	0.48
5:A:1:PHE:HA	5:A:389:GLN:HB2	1.95	0.48
6:B:217:ASP:OD2	6:B:255:HIS:NE2	2.46	0.48
3:3:123:ILE:HD11	3:3:184:VAL:CG2	2.44	0.48
1:1:53:LEU:HD11	1:1:76:LEU:CD1	2.44	0.48
3:3:120:ARG:HD3	3:3:146:GLU:OE2	2.14	0.47
6:B:71:SER:HG	6:B:82:VAL:H	1.59	0.47
2:2:87:HIS:CE1	2:2:91:TYR:HB3	2.49	0.47
6:B:74:ARG:NH2	6:B:146:LEU:H	2.11	0.47
5:A:50:ILE:HD11	5:A:76:GLY:HA2	1.96	0.47
5:A:458:ASN:ND2	8:A:607:NAG:H82	2.28	0.47
6:B:362:ASP:HA	6:B:413:ILE:HG12	1.97	0.47
3:3:217:ALA:O	3:3:218:ARG:HB2	2.15	0.47
1:1:142:THR:CB	5:A:150:ASP:CB	2.88	0.47
6:B:319:GLU:HG3	6:B:330:VAL:HG21	1.97	0.47
3:3:76:GLN:HG3	3:3:185:CYS:SG	2.55	0.47
1:1:136:TYR:C	2:2:80:LEU:O	2.50	0.47
3:3:19:PRO:HB3	4:4:18:THR:HA	1.98	0.46
2:2:87:HIS:CE1	2:2:89:GLY:HA3	2.50	0.46
3:3:212:ARG:CZ	3:3:213:LEU:HD13	2.45	0.46
6:B:180:ILE:O	6:B:182:TYR:N	2.49	0.46
6:B:436:CYS:HB2	6:B:456:CYS:HA	1.96	0.46
1:1:41:LYS:HA	1:1:177:LEU:HD23	1.96	0.46
1:1:145:ARG:N	5:A:178:TYR:CE2	2.69	0.46
6:B:353:SER:HB2	6:B:389:MET:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:59:HIS:HA	3:3:220:GLN:CB	2.41	0.46
3:3:63:TYR:HB3	3:3:200:VAL:HG12	1.98	0.46
1:1:138:GLU:H	2:2:80:LEU:H	1.63	0.46
3:3:79:LEU:CD1	3:3:159:ILE:HG21	2.46	0.46
4:4:22:ILE:O	4:4:22:ILE:HD12	2.16	0.46
1:1:134:CYS:SG	1:1:156:ALA:CA	3.04	0.46
1:1:77:GLU:OE1	1:1:181:LYS:CE	2.63	0.46
6:B:308:PHE:HB2	6:B:330:VAL:HG12	1.98	0.46
6:B:138:ARG:HB3	6:B:341:LEU:HD11	1.98	0.46
3:3:55:LEU:HD11	3:3:203:ALA:HB2	1.98	0.46
5:A:494:GLN:NE2	8:A:611:NAG:H3	2.31	0.46
6:B:84:ILE:HG13	6:B:105:VAL:HG22	1.98	0.46
3:3:40:ARG:HB3	4:4:66:ASP:HB2	1.98	0.45
5:A:116:THR:HG23	5:A:147:ILE:HG21	1.97	0.45
1:1:53:LEU:HD13	1:1:165:TYR:CE1	2.51	0.45
2:2:100:TYR:HE1	2:2:170:GLN:HE21	1.65	0.45
2:2:99:ALA:HA	2:2:214:PHE:HE2	1.80	0.45
7:A:614:MAN:H62	7:A:615:MAN:O5	2.17	0.45
1:1:5:GLY:HA2	3:3:154:LYS:HB2	1.97	0.45
2:2:189:VAL:HG11	2:2:195:PRO:HA	1.99	0.45
5:A:455:ASN:HA	5:A:593:LEU:HD11	1.97	0.45
6:B:448:HIS:O	6:B:451:ASN:ND2	2.35	0.45
3:3:79:LEU:HD22	3:3:125:TYR:CE1	2.51	0.45
8:A:607:NAG:HO3	8:A:608:NAG:C1	2.30	0.45
1:1:194:ILE:HG12	3:3:219:THR:OG1	2.16	0.45
2:2:90:VAL:O	2:2:94:LEU:HD13	2.17	0.45
6:B:363:THR:HG22	6:B:365:GLY:H	1.82	0.45
8:A:607:NAG:O3	8:A:608:NAG:C1	2.65	0.45
1:1:144:VAL:HG13	1:1:148:LEU:HB3	1.99	0.44
3:3:44:PHE:O	3:3:47:VAL:HG22	2.16	0.44
6:B:18:LEU:HD13	6:B:58:PRO:HG3	1.99	0.44
1:1:59:HIS:HA	3:3:220:GLN:H	1.82	0.44
1:1:65:LEU:O	1:1:68:THR:OG1	2.31	0.44
6:B:261:LYS:HG2	6:B:266:VAL:HG12	1.98	0.44
1:1:143:ASN:HD21	5:A:148:ASP:CG	2.10	0.44
5:A:253:VAL:HB	5:A:267:PHE:HB2	1.99	0.44
5:A:569:ALA:HB1	5:A:573:GLY:HA2	1.99	0.44
1:1:148:LEU:CD1	6:B:216:ILE:HG23	2.47	0.44
6:B:111:TYR:CD1	6:B:352:ARG:HB2	2.39	0.44
6:B:123:ALA:HB2	6:B:214:ALA:HB2	1.98	0.44
2:2:43:VAL:HG11	2:2:209:HIS:CD2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:242:GLY:HA2	5:A:253:VAL:HG22	1.99	0.44
5:A:47:GLN:HA	5:A:48:PRO:HD3	1.90	0.44
3:3:104:THR:HG21	3:3:158:SER:HB3	2.00	0.44
5:A:554:PRO:HB3	5:A:591:HIS:CE1	2.52	0.44
2:2:189:VAL:O	2:2:189:VAL:HG23	2.17	0.44
1:1:138:GLU:OE1	2:2:79:HIS:CB	2.66	0.44
1:1:135:LYS:HA	1:1:140:HIS:HE1	1.83	0.43
1:1:144:VAL:HG11	1:1:152:ALA:HB2	2.00	0.43
5:A:569:ALA:HB2	5:A:575:GLN:HG2	2.00	0.43
6:B:94:ARG:HD2	6:B:95:PRO:HD2	2.00	0.43
1:1:136:TYR:H	1:1:137:GLY:HA2	1.82	0.43
5:A:373:VAL:HB	5:A:391:LEU:HB2	2.00	0.43
6:B:197:THR:OG1	6:B:198:ASN:N	2.51	0.43
3:3:172:SER:HA	3:3:179:ASN:HB2	2.01	0.43
1:1:154:LYS:O	1:1:155:VAL:C	2.57	0.43
1:1:142:THR:CA	5:A:150:ASP:CB	2.96	0.43
1:1:137:GLY:N	2:2:80:LEU:O	2.52	0.42
1:1:134:CYS:C	2:2:82:GLU:OE2	2.48	0.42
6:B:312:GLN:HA	6:B:315:VAL:HG23	2.01	0.42
3:3:218:ARG:HG2	3:3:219:THR:H	1.84	0.42
3:3:73:ILE:HD11	3:3:134:LYS:O	2.19	0.42
1:1:64:ALA:HB2	3:3:220:GLN:HG3	2.01	0.42
1:1:137:GLY:HA3	2:2:80:LEU:CB	2.48	0.42
3:3:123:ILE:O	3:3:123:ILE:HG23	2.19	0.42
6:B:71:SER:OG	6:B:82:VAL:N	2.41	0.42
2:2:103:ASN:CB	2:2:208:VAL:HG12	2.49	0.42
2:2:6:GLU:HG3	2:2:8:THR:H	1.84	0.42
5:A:364:TYR:HB3	5:A:369:LYS:HE2	2.02	0.42
3:3:74:LEU:HD11	3:3:188:GLN:HB2	2.00	0.42
5:A:449:VAL:HG21	5:A:557:ILE:HD13	2.01	0.42
2:2:6:GLU:HG2	2:2:10:LEU:HG	2.02	0.42
6:B:258:MET:SD	6:B:258:MET:N	2.93	0.42
3:3:219:THR:O	3:3:220:GLN:C	2.58	0.42
6:B:118:LEU:HD11	6:B:225:ALA:HB1	2.01	0.42
6:B:429:SER:HA	6:B:430:PRO:HD3	1.85	0.42
1:1:134:CYS:HG	1:1:156:ALA:HB1	1.64	0.41
6:B:244:HIS:HB2	6:B:304:VAL:HA	2.02	0.41
1:1:61:LEU:HD13	3:3:97:TYR:HB3	2.01	0.41
5:A:518:SER:HA	5:A:519:PRO:HD3	1.87	0.41
3:3:119:ALA:HA	3:3:191:HIS:HA	2.02	0.41
5:A:350:LEU:HA	5:A:420:PRO:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:157:ARG:HD2	1:1:157:ARG:HA	1.85	0.41
6:B:151:ARG:NH2	6:B:239:ARG:HG2	2.35	0.41
2:2:169:ASP:OD1	2:2:170:GLN:N	2.52	0.41
5:A:149:ALA:H	5:A:154:PHE:HD1	1.67	0.41
6:B:223:PHE:HB3	6:B:290:PRO:HG2	2.01	0.41
1:1:39:PHE:HA	1:1:178:TYR:O	2.21	0.41
1:1:131:ASN:ND2	2:2:129:LEU:N	2.66	0.41
1:1:132:GLY:CA	1:1:157:ARG:HG3	2.48	0.41
1:1:97:ALA:C	1:1:99:ASP:H	2.24	0.41
4:4:66:ASP:O	4:4:70:LYS:HE2	2.21	0.41
6:B:435:ASP:HA	6:B:438:LYS:NZ	2.36	0.41
5:A:436:ARG:HH12	5:A:572:THR:HG1	1.62	0.41
5:A:463:LEU:HD21	5:A:517:ARG:HE	1.86	0.41
8:A:612:NAG:HO3	8:A:613:NAG:C1	2.25	0.41
6:B:171:GLU:H	6:B:171:GLU:CD	2.25	0.41
3:3:55:LEU:HB2	3:3:201:VAL:HG13	2.03	0.41
5:A:164:THR:HB	5:A:237:ASP:HB2	2.03	0.41
5:A:458:ASN:ND2	8:A:607:NAG:C7	2.84	0.41
1:1:135:LYS:CE	2:2:129:LEU:CG	2.88	0.40
5:A:196:ASP:HB3	5:A:199:VAL:HB	2.03	0.40
5:A:575:GLN:HA	5:A:576:PRO:HD3	1.91	0.40
1:1:46:ASP:O	1:1:173:VAL:HG12	2.20	0.40
2:2:121:LEU:HB2	2:2:148:ILE:HB	2.04	0.40
3:3:32:PRO:HA	3:3:33:PRO:HD3	1.96	0.40
5:A:371:GLY:HA3	5:A:404:PHE:HB3	2.02	0.40
1:1:147:ASP:N	6:B:218:THR:CB	2.82	0.40
6:B:51:GLN:O	6:B:55:ILE:HG13	2.21	0.40
6:B:71:SER:HB2	6:B:75:GLN:NE2	2.36	0.40
2:2:100:TYR:HB3	2:2:168:TYR:HB3	2.04	0.40
2:2:137:LEU:HB3	2:2:182:MET:SD	2.61	0.40
6:B:152:LEU:O	6:B:196:LEU:HA	2.21	0.40
6:B:15:GLU:HG3	6:B:432:CYS:O	2.21	0.40
1:1:147:ASP:CA	6:B:218:THR:HA	2.51	0.40
2:2:112:VAL:HG12	2:2:154:MET:SD	2.62	0.40
3:3:74:LEU:CD1	3:3:188:GLN:HB2	2.52	0.40
1:1:134:CYS:CB	1:1:156:ALA:CB	2.93	0.40
5:A:156:GLN:OE1	6:B:164:PRO:HG3	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	1	208/210 (99%)	192 (92%)	15 (7%)	1 (0%)	32	74
2	2	212/214 (99%)	199 (94%)	13 (6%)	0	100	100
3	3	218/220 (99%)	203 (93%)	15 (7%)	0	100	100
4	4	43/70 (61%)	39 (91%)	4 (9%)	0	100	100
5	A	581/594 (98%)	550 (95%)	27 (5%)	4 (1%)	25	68
6	B	434/470 (92%)	397 (92%)	32 (7%)	5 (1%)	15	57
All	All	1696/1778 (95%)	1580 (93%)	106 (6%)	10 (1%)	33	71

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	B	375	ASN
5	A	149	ALA
5	A	571	THR
5	A	28	PRO
6	B	9	GLY
1	1	158	THR
5	A	516	SER
6	B	124	SER
6	B	181	PRO
6	B	391	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	1	177/177 (100%)	176 (99%)	1 (1%)	89	94
2	2	186/188 (99%)	186 (100%)	0	100	100
3	3	176/176 (100%)	176 (100%)	0	100	100
4	4	37/57 (65%)	37 (100%)	0	100	100
5	A	483/487 (99%)	472 (98%)	11 (2%)	56	79
6	B	394/410 (96%)	377 (96%)	17 (4%)	33	64
All	All	1453/1495 (97%)	1424 (98%)	29 (2%)	63	82

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	131	ASN
5	A	116	THR
5	A	119	LYS
5	A	145	GLN
5	A	147	ILE
5	A	183	LEU
5	A	275	TYR
5	A	368	ASP
5	A	494	GLN
5	A	512	LEU
5	A	538	LEU
5	A	593	LEU
6	B	61	GLN
6	B	72	VAL
6	B	77	ASN
6	B	91	LEU
6	B	131	THR
6	B	145	LYS
6	B	163	SER
6	B	196	LEU
6	B	209	ASN
6	B	215	ASN
6	B	246	LEU
6	B	261	LYS
6	B	319	GLU
6	B	341	LEU
6	B	408	ARG
6	B	416	LYS
6	B	430	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	131	ASN
3	3	76	GLN
5	A	524	ASN
6	B	215	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](#)

Of 26 ligands modelled in this entry, 4 are monoatomic - leaving 22 for Mogul analysis.

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	$\# Z > 2$
7	MAN	1	301	-	11,11,12	0.57	0	13,15,17	2.39	6 (46%)
7	MAN	1	302	-	11,11,12	0.63	0	13,15,17	2.47	6 (46%)
7	MAN	2	301	7	11,11,12	0.54	0	13,15,17	2.04	5 (38%)
7	MAN	2	302	7	11,11,12	0.62	0	13,15,17	2.02	5 (38%)
7	MAN	3	301	-	11,11,12	0.61	0	13,15,17	2.57	3 (23%)
8	NAG	A	601	8	14,14,15	0.48	0	15,19,21	0.61	0
8	NAG	A	602	8,7	14,14,15	0.48	0	15,19,21	0.68	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	MAN	A	603	8	12,12,12	0.42	0	17,17,17	0.53	0
8	NAG	A	604	-	14,14,15	0.47	0	15,19,21	2.60	3 (20%)
8	NAG	A	605	7	14,14,15	0.50	0	15,19,21	1.20	2 (13%)
7	MAN	A	606	8	11,11,12	0.65	0	13,15,17	1.50	3 (23%)
8	NAG	A	607	8,5	14,14,15	0.25	0	15,19,21	0.53	0
8	NAG	A	608	8,7	14,14,15	0.26	0	15,19,21	0.53	0
7	MAN	A	609	8,7	11,11,12	0.25	0	13,15,17	0.45	0
7	MAN	A	610	7	11,11,12	0.24	0	13,15,17	0.44	0
8	NAG	A	611	-	14,14,15	0.28	0	15,19,21	0.53	0
8	NAG	A	612	8	14,14,15	0.27	0	15,19,21	0.51	0
8	NAG	A	613	8,7	14,14,15	0.33	0	15,19,21	0.61	0
7	MAN	A	614	8,7	12,12,12	0.46	0	17,17,17	0.62	0
7	MAN	A	615	7	12,12,12	0.42	0	17,17,17	0.55	0
8	NAG	B	501	6	14,14,15	0.53	0	15,19,21	0.55	0
8	NAG	B	502	-	14,14,15	0.47	0	15,19,21	0.69	0

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
7	MAN	1	301	-	-	0/2/19/22	0/1/1/1
7	MAN	1	302	-	-	0/2/19/22	0/1/1/1
7	MAN	2	301	7	-	0/2/19/22	0/1/1/1
7	MAN	2	302	7	-	0/2/19/22	0/1/1/1
7	MAN	3	301	-	-	0/2/19/22	0/1/1/1
8	NAG	A	601	8	-	0/6/23/26	0/1/1/1
8	NAG	A	602	8,7	-	0/6/23/26	0/1/1/1
7	MAN	A	603	8	-	0/2/22/22	0/1/1/1
8	NAG	A	604	-	-	0/6/23/26	0/1/1/1
8	NAG	A	605	7	-	0/6/23/26	0/1/1/1
7	MAN	A	606	8	1/1/4/5	0/2/19/22	0/1/1/1
8	NAG	A	607	8,5	-	0/6/23/26	0/1/1/1
8	NAG	A	608	8,7	-	0/6/23/26	0/1/1/1
7	MAN	A	609	8,7	-	0/2/19/22	0/1/1/1
7	MAN	A	610	7	1/1/4/5	0/2/19/22	0/1/1/1
8	NAG	A	611	-	-	0/6/23/26	0/1/1/1
8	NAG	A	612	8	-	0/6/23/26	0/1/1/1
8	NAG	A	613	8,7	-	0/6/23/26	0/1/1/1
7	MAN	A	614	8,7	-	0/2/22/22	0/1/1/1
7	MAN	A	615	7	-	0/2/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	B	501	6	1/1/5/7	0/6/23/26	0/1/1/1
8	NAG	B	502	-	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	604	NAG	O5-C1-C2	-8.50	99.65	111.47
7	1	301	MAN	C6-C5-C4	-5.09	101.09	113.00
7	2	301	MAN	O4-C4-C3	-4.23	101.16	110.36
7	3	301	MAN	C2-C3-C4	-4.00	103.90	110.88
7	1	301	MAN	O4-C4-C3	-3.73	102.25	110.36
7	2	302	MAN	O4-C4-C3	-3.67	102.38	110.36
7	3	301	MAN	O5-C1-C2	-3.42	105.42	110.79
7	1	301	MAN	C3-C4-C5	-3.14	104.68	110.22
7	1	301	MAN	O2-C2-C3	-2.95	104.39	110.17
8	A	605	NAG	O5-C1-C2	-2.81	107.56	111.47
8	A	604	NAG	O7-C7-C8	-2.74	117.07	122.06
8	A	604	NAG	C4-C3-C2	-2.68	107.09	111.02
7	A	606	MAN	O4-C4-C5	-2.60	102.74	109.28
7	2	301	MAN	O3-C3-C2	-2.40	105.66	110.02
7	A	606	MAN	C6-C5-C4	-2.39	107.42	113.00
7	1	302	MAN	O4-C4-C3	-2.17	105.64	110.36
8	A	605	NAG	C4-C3-C2	-2.17	107.84	111.02
7	1	302	MAN	C1-C2-C3	-2.11	106.97	109.65
7	2	301	MAN	O3-C3-C4	2.03	114.78	110.36
7	1	301	MAN	C2-C3-C4	2.12	114.58	110.88
7	2	301	MAN	C1-O5-C5	2.15	115.14	112.17
7	2	302	MAN	C1-O5-C5	2.27	115.29	112.17
7	1	301	MAN	O2-C2-C1	2.40	114.05	109.18
7	2	302	MAN	O5-C1-C2	2.52	114.73	110.79
7	2	302	MAN	O3-C3-C2	2.58	114.72	110.02
7	1	302	MAN	O4-C4-C5	2.78	116.30	109.28
7	1	302	MAN	O2-C2-C1	2.97	115.21	109.18
7	A	606	MAN	O2-C2-C3	2.99	116.04	110.17
7	2	301	MAN	O4-C4-C5	3.12	117.16	109.28
7	2	302	MAN	C2-C3-C4	3.22	116.49	110.88
7	1	302	MAN	C3-C4-C5	3.44	116.27	110.22
7	1	302	MAN	C1-O5-C5	5.75	120.09	112.17
7	3	301	MAN	C1-C2-C3	6.73	118.19	109.65

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	A	610	MAN	C1
8	B	501	NAG	C1
7	A	606	MAN	C1

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 38 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	602	NAG	1	0
7	A	603	MAN	1	0
8	A	607	NAG	8	0
8	A	608	NAG	4	0
8	A	611	NAG	3	0
8	A	612	NAG	20	0
8	A	613	NAG	9	0
7	A	614	MAN	6	0
7	A	615	MAN	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
6	B	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	351:LEU	C	352:ARG	N	15.18
1	B	110:ASP	C	111:TYR	N	8.73