



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2018 – 09:30 pm GMT

PDB ID : 4MMX  
Title : Integrin AlphaVBeta3 ectodomain bound to the tenth domain of Fibronectin  
Authors : van Agthoven, J.; Xiong, J.; Arnaout, M.A.  
Deposited on : 2013-09-09  
Resolution : 3.32 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk31020  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk31020

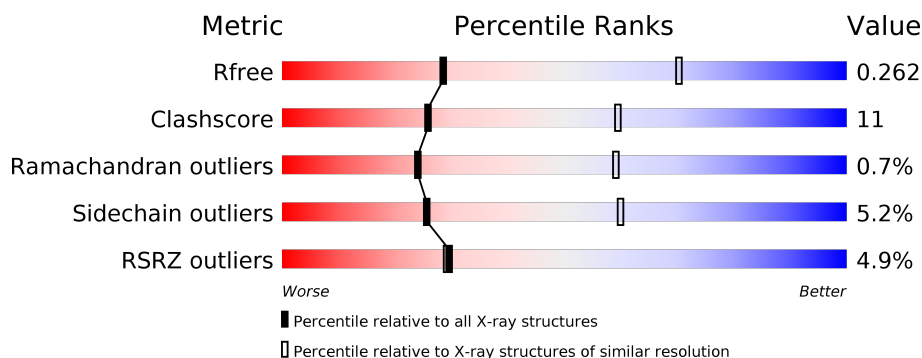
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.32 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	111664	1128 (3.38-3.26)
Clashscore	122126	1187 (3.38-3.26)
Ramachandran outliers	120053	1167 (3.38-3.26)
Sidechain outliers	120020	1166 (3.38-3.26)
RSRZ outliers	108989	1094 (3.38-3.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	959	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 72%, yellow 23%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> <span>%</span> <span>72%</span> <span>23%</span> <span>• •</span> </div> </div>
2	B	692	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 4%, green 74%, yellow 24%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> <span>4%</span> <span>74%</span> <span>24%</span> <span>•</span> </div> </div>
3	C	98	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 41%, green 56%, yellow 34%, orange 5%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> <span>41%</span> <span>56%</span> <span>34%</span> <span>5%</span> <span>5%</span> </div> </div>

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
4	NAG	A	1025	-	-	-	X
5	BMA	A	1026	-	-	-	X
6	MAN	A	1004	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 13626 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Integrin alpha-V.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	924	Total	C	N	O	S	0	0	0
			7196	4556	1221	1384	35			

- Molecule 2 is a protein called Integrin beta-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	690	Total	C	N	O	S	0	0	0
			5294	3250	904	1070	70			

- Molecule 3 is a protein called Fibronectin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	93	Total	C	N	O	0	0	0
			694	438	115	141			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1510	GLY	-	EXPRESSION TAG	UNP P02751
C	1511	LYS	-	EXPRESSION TAG	UNP P02751
C	1512	LYS	-	EXPRESSION TAG	UNP P02751
C	1513	GLY	-	EXPRESSION TAG	UNP P02751
C	1514	LYS	-	EXPRESSION TAG	UNP P02751

- Molecule 4 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



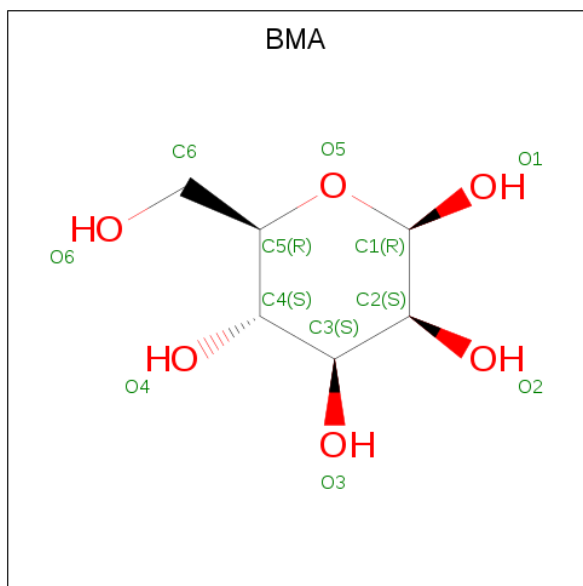
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is BETA-D-MANNOSE (three-letter code: BMA) (formula:  $C_6H_{12}O_6$ ).



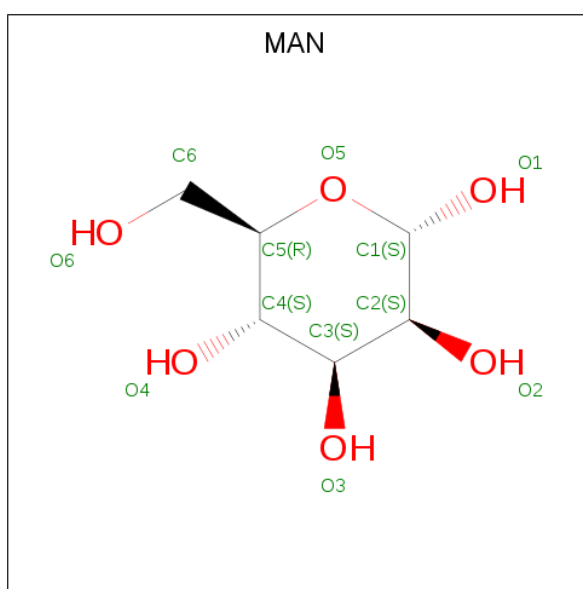
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		
5	B	1	Total	C	O	0	0
			11	6	5		

- Molecule 6 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			11	6	5		
6	A	1	Total	C	O	0	0
			11	6	5		
6	A	1	Total	C	O	0	0
			11	6	5		
6	A	1	Total	C	O	0	0
			11	6	5		

- Molecule 7 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	3	Total	Mn	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	5	Total	Mn	0	0
			5	5		

- Molecule 8 is water.

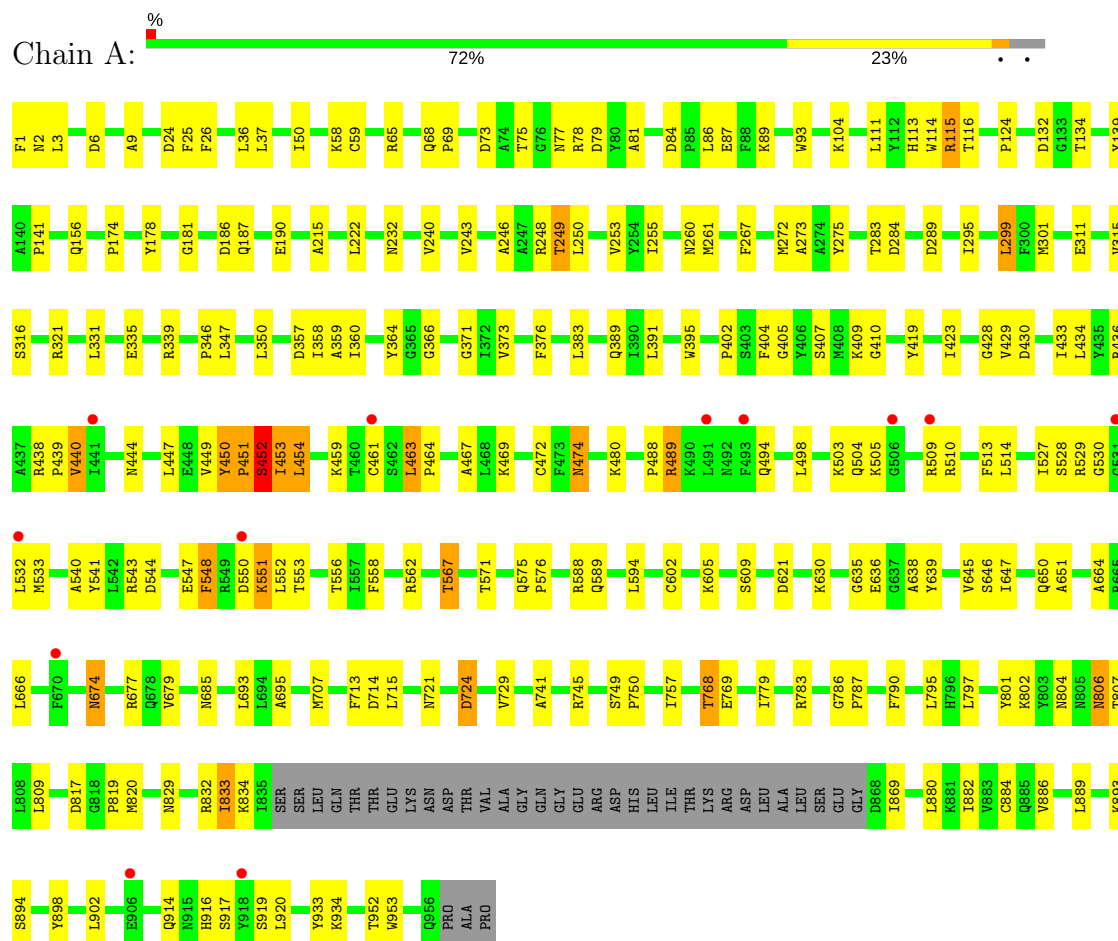
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	2	Total	O	0	0
			2	2		

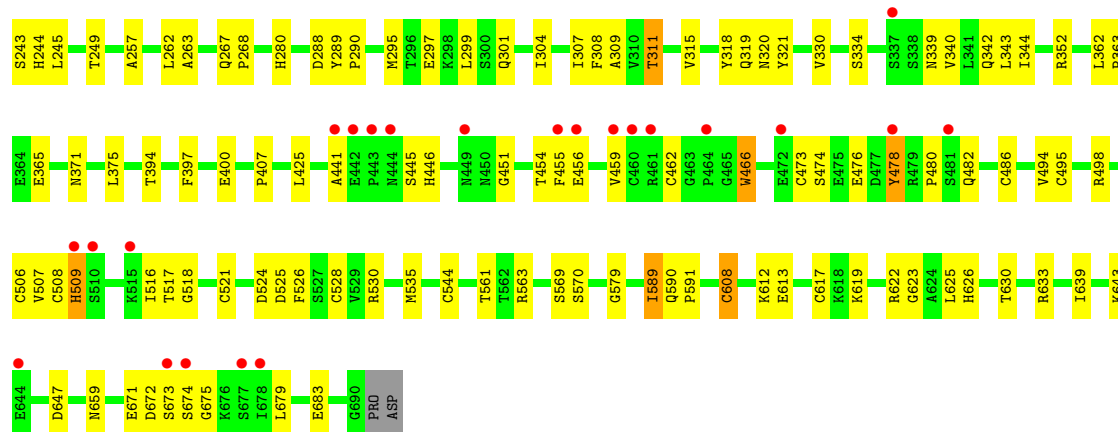


### 3 Residue-property plots

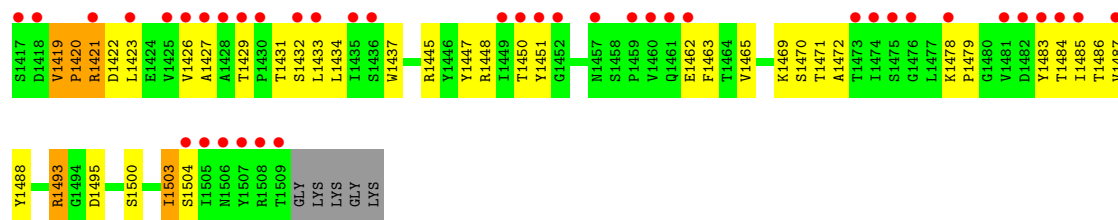
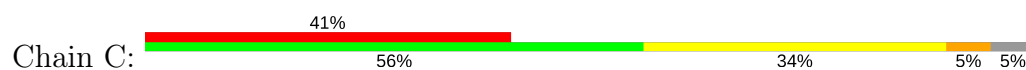
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

#### • Molecule 1: Integrin alpha-V





### • Molecule 3: Fibronectin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	129.86Å 129.86Å 305.83Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.51 – 3.32 42.51 – 3.32	Depositor EDS
% Data completeness (in resolution range)	88.0 (42.51-3.32) 88.0 (42.51-3.32)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.73 (at 3.32Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.208 , 0.259 0.212 , 0.262	Depositor DCC
$R_{free}$ test set	1943 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	86.7	Xtriage
Anisotropy	0.148	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 50.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.036 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	13626	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, MN, 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  >5	RMSZ	# Z  >5
1	A	0.23	0/7352	0.44	1/9967 (0.0%)
2	B	0.26	0/5390	0.48	0/7289
3	C	0.28	0/710	0.57	0/975
All	All	0.24	0/13452	0.46	1/18231 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	450	TYR	C-N-CD	-8.01	102.97	120.60

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	7196	0	7013	156	0
2	B	5294	0	5024	115	0
3	C	694	0	688	35	0
4	A	238	0	210	3	0
4	B	84	0	75	4	0
5	A	55	0	45	4	0
5	B	11	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	44	0	40	1	0
7	A	5	0	0	0	0
7	B	3	0	0	0	0
8	B	2	0	0	0	0
All	All	13626	0	13105	301	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 11.

All (301) 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:B:162:SER:CB	2:B:163:PRO:HD2	1.47	1.33
2:B:162:SER:HB3	2:B:163:PRO:CD	1.66	1.25
1:A:450:TYR:HB3	1:A:451:PRO:CD	1.69	1.21
1:A:454:LEU:HD23	1:A:454:LEU:N	1.50	1.16
3:C:1419:VAL:HG22	3:C:1420:PRO:HD2	1.17	1.13
1:A:450:TYR:HB3	1:A:451:PRO:HD2	1.12	1.11
3:C:1421:ARG:HG2	3:C:1422:ASP:H	1.16	1.07
2:B:162:SER:CB	2:B:163:PRO:CD	2.30	1.05
2:B:162:SER:HB3	2:B:163:PRO:HD2	1.03	1.00
2:B:162:SER:HB2	2:B:163:PRO:HD2	1.46	0.98
1:A:454:LEU:CD2	1:A:454:LEU:N	2.30	0.94
1:A:450:TYR:CB	1:A:451:PRO:HD2	1.99	0.93
1:A:450:TYR:CB	1:A:451:PRO:CD	2.50	0.89
3:C:1419:VAL:HG23	3:C:1500:SER:OG	1.74	0.88
1:A:488:PRO:HG2	1:A:567:THR:HG22	1.57	0.86
3:C:1419:VAL:CG2	3:C:1420:PRO:HD2	2.03	0.85
2:B:161:VAL:O	2:B:162:SER:O	1.94	0.84
1:A:453:ILE:C	1:A:454:LEU:HD23	1.98	0.83
1:A:449:VAL:CG1	1:A:449:VAL:O	2.30	0.79
2:B:623:GLY:HA2	2:B:626:HIS:HB3	1.63	0.78
3:C:1421:ARG:HG2	3:C:1422:ASP:N	1.97	0.78
1:A:453:ILE:HD11	1:A:639:TYR:CE2	2.18	0.77
3:C:1419:VAL:HG23	3:C:1500:SER:CB	2.14	0.76
1:A:450:TYR:HB3	1:A:451:PRO:HD3	1.66	0.76
1:A:453:ILE:HG22	1:A:453:ILE:O	1.84	0.75
2:B:161:VAL:HG23	2:B:162:SER:N	1.99	0.75
1:A:480:LYS:HB2	1:A:533:MET:HG2	1.69	0.75
1:A:450:TYR:O	1:A:451:PRO:C	2.25	0.75
1:A:504:GLN:HG2	1:A:509:ARG:HG3	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1421:ARG:CG	3:C:1422:ASP:H	2.00	0.72
1:A:449:VAL:O	1:A:449:VAL:HG13	1.88	0.72
3:C:1451:TYR:HB3	3:C:1485:ILE:HG23	1.72	0.71
2:B:27:SER:HB2	2:B:53:SER:HB3	1.71	0.71
1:A:347:LEU:HD11	1:A:357:ASP:HB2	1.72	0.71
1:A:187:GLN:HB2	1:A:190:GLU:HB2	1.74	0.70
1:A:609:SER:HB3	1:A:630:LYS:HB3	1.73	0.69
2:B:168:SER:HB2	2:B:169:PRO:HD2	1.75	0.68
2:B:590:GLN:HG2	2:B:591:PRO:HD2	1.76	0.68
1:A:402:PRO:HA	1:A:428:GLY:HA3	1.75	0.68
1:A:779:ILE:HD12	1:A:898:TYR:HD2	1.59	0.68
3:C:1419:VAL:CG2	3:C:1500:SER:OG	2.42	0.68
3:C:1421:ARG:HB2	3:C:1503:ILE:HD12	1.76	0.68
2:B:134:LEU:O	2:B:138:LEU:N	2.20	0.67
3:C:1419:VAL:HG22	3:C:1420:PRO:CD	2.11	0.67
1:A:459:LYS:HB3	1:A:469:LYS:HB3	1.77	0.67
1:A:505:LYS:HB3	2:B:509:HIS:CD2	2.29	0.67
2:B:162:SER:HB3	2:B:163:PRO:HD3	1.74	0.67
1:A:556:THR:HG22	1:A:589:GLN:HG2	1.76	0.66
2:B:486:CYS:HB3	2:B:495:CYS:HB3	1.78	0.66
1:A:707:MET:HE2	1:A:934:LYS:H	1.61	0.66
3:C:1448:ARG:HB2	3:C:1488:TYR:HB2	1.78	0.66
1:A:802:LYS:HG2	1:A:807:THR:HA	1.78	0.66
1:A:450:TYR:CZ	5:A:1015:BMA:O2	2.47	0.65
1:A:450:TYR:O	1:A:452:SER:N	2.30	0.65
2:B:622:ARG:HH22	2:B:659:ASN:HD22	1.44	0.65
1:A:474:ASN:OD1	1:A:474:ASN:N	2.28	0.65
2:B:83:VAL:O	2:B:86:GLN:NE2	2.30	0.64
1:A:438:ARG:NE	1:A:575:GLN:O	2.25	0.63
1:A:503:LYS:HG3	1:A:510:ARG:HD3	1.81	0.63
2:B:163:PRO:O	2:B:164:TYR:C	2.36	0.63
1:A:769:GLU:HG2	1:A:902:LEU:HD11	1.79	0.63
2:B:498:ARG:HD3	2:B:516:ILE:HD13	1.81	0.63
2:B:162:SER:O	2:B:163:PRO:C	2.37	0.62
3:C:1419:VAL:HG23	3:C:1500:SER:HB2	1.82	0.62
1:A:551:LYS:HB3	1:A:553:THR:H	1.64	0.62
2:B:134:LEU:O	2:B:137:LYS:N	2.33	0.62
2:B:164:TYR:O	2:B:215:ASN:HB2	2.00	0.62
3:C:1448:ARG:NH2	3:C:1462:GLU:OE1	2.28	0.61
1:A:664:ALA:HB3	1:A:695:ALA:HB2	1.82	0.61
1:A:249:THR:HG23	1:A:273:ALA:H	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:VAL:HG22	1:A:255:ILE:HG12	1.81	0.60
2:B:71:ASP:OD1	2:B:71:ASP:N	2.33	0.60
1:A:552:LEU:HD21	1:A:594:LEU:HD22	1.83	0.60
2:B:8:ARG:NH2	2:B:544:CYS:SG	2.74	0.60
1:A:544:ASP:HB3	1:A:547:GLU:HG3	1.84	0.60
1:A:450:TYR:CE1	5:A:1015:BMA:O2	2.54	0.60
1:A:395:TRP:HB3	1:A:429:VAL:HG11	1.81	0.60
1:A:395:TRP:HE1	1:A:433:ILE:HD11	1.65	0.60
1:A:464:PRO:HD2	1:A:467:ALA:HA	1.83	0.59
2:B:507:VAL:HB	2:B:509:HIS:HE1	1.64	0.59
1:A:1:PHE:HA	1:A:389:GLN:HB2	1.85	0.59
1:A:371:GLY:HA3	1:A:404:PHE:HB3	1.85	0.59
3:C:1429:THR:OG1	3:C:1431:THR:O	2.21	0.58
1:A:347:LEU:HD23	1:A:359:ALA:HB2	1.86	0.58
2:B:617:CYS:HB2	2:B:625:LEU:HB3	1.86	0.58
1:A:447:LEU:O	1:A:588:ARG:NE	2.35	0.58
1:A:645:VAL:HB	1:A:679:VAL:HB	1.86	0.58
3:C:1426:VAL:HB	3:C:1434:LEU:HD23	1.84	0.58
1:A:472:CYS:HA	1:A:541:TYR:HA	1.86	0.58
2:B:643:LYS:HA	2:B:683:GLU:HG2	1.85	0.58
1:A:741:ALA:H	1:A:786:GLY:HA3	1.69	0.57
2:B:25:TRP:HB3	2:B:55:GLU:HB2	1.86	0.57
1:A:674:ASN:HD22	4:A:1020:NAG:H61	1.68	0.57
1:A:347:LEU:HD13	1:A:350:LEU:HB2	1.87	0.57
1:A:768:THR:HG23	1:A:834:LYS:HB2	1.87	0.57
1:A:373:VAL:HB	1:A:391:LEU:HB2	1.84	0.57
1:A:453:ILE:CG2	1:A:453:ILE:O	2.52	0.57
1:A:50:ILE:HD12	1:A:89:LYS:HB2	1.86	0.57
2:B:217:ASP:OD1	2:B:219:PRO:O	2.23	0.57
2:B:163:PRO:O	2:B:165:MET:N	2.38	0.56
2:B:133:ASN:O	2:B:204:ASN:ND2	2.38	0.56
1:A:801:TYR:HB2	1:A:880:LEU:HB2	1.86	0.56
2:B:613:GLU:HG2	2:B:625:LEU:HB2	1.88	0.56
2:B:466:TRP:O	2:B:473:CYS:HB2	2.06	0.56
3:C:1450:THR:O	3:C:1486:THR:N	2.38	0.56
1:A:463:LEU:HA	1:A:467:ALA:HB2	1.87	0.56
1:A:215:ALA:HB3	3:C:1445:ARG:HD3	1.87	0.55
1:A:36:LEU:HB2	1:A:59:CYS:HB2	1.88	0.55
3:C:1432:SER:OG	3:C:1433:LEU:N	2.38	0.55
2:B:509:HIS:N	2:B:509:HIS:ND1	2.54	0.55
1:A:114:TRP:CE2	1:A:116:THR:HA	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:446:HIS:HA	2:B:451:GLY:HA2	1.88	0.54
2:B:639:ILE:HG12	2:B:679:LEU:HD23	1.88	0.54
2:B:339:ASN:CG	2:B:340:VAL:H	2.11	0.54
1:A:9:ALA:HB3	1:A:434:LEU:HB3	1.89	0.54
1:A:621:ASP:HB2	1:A:787:PRO:HB3	1.89	0.54
3:C:1437:TRP:O	3:C:1470:SER:OG	2.26	0.54
1:A:181:GLY:HA3	1:A:222:LEU:HB3	1.90	0.53
2:B:215:ASN:O	3:C:1495:ASP:HB3	2.09	0.53
1:A:250:LEU:HD12	1:A:272:MET:HG2	1.90	0.53
2:B:160:PRO:C	2:B:161:VAL:HG13	2.29	0.53
2:B:319:GLN:HA	2:B:330:VAL:HG21	1.91	0.53
2:B:579:GLY:HA2	2:B:589:ILE:HG13	1.89	0.53
1:A:178:TYR:CD2	3:C:1493:ARG:HG2	2.44	0.52
2:B:498:ARG:O	2:B:508:CYS:HB3	2.09	0.52
1:A:498:LEU:HB2	1:A:558:PHE:HB3	1.89	0.52
1:A:73:ASP:OD2	1:A:75:THR:OG1	2.21	0.52
2:B:23:CYS:HA	2:B:40:LEU:HB3	1.92	0.52
1:A:24:ASP:OD1	1:A:25:PHE:N	2.38	0.52
2:B:340:VAL:HA	2:B:343:LEU:HD23	1.91	0.52
3:C:1478:LYS:HE3	3:C:1479:PRO:HD2	1.90	0.52
1:A:243:VAL:HG22	1:A:246:ALA:HB2	1.91	0.51
2:B:673:SER:C	2:B:675:GLY:H	2.13	0.51
1:A:914:GLN:O	1:A:953:TRP:NE1	2.43	0.51
1:A:513:PHE:HA	1:A:540:ALA:HA	1.93	0.51
1:A:646:SER:HB2	1:A:714:ASP:HB2	1.92	0.51
2:B:530:ARG:HG2	2:B:535:MET:HA	1.92	0.51
1:A:423:ILE:HG12	1:A:434:LEU:HD23	1.93	0.51
1:A:589:GLN:OE1	1:A:685:ASN:ND2	2.44	0.51
2:B:136:THR:H	2:B:204:ASN:HD21	1.59	0.51
1:A:248:ARG:HG3	1:A:250:LEU:HD13	1.92	0.50
1:A:2:ASN:OD1	1:A:2:ASN:N	2.43	0.50
2:B:245:LEU:HD22	2:B:307:ILE:HD11	1.93	0.50
2:B:400:GLU:HB2	4:B:703:NAG:H83	1.92	0.50
1:A:674:ASN:ND2	4:A:1020:NAG:H61	2.27	0.50
1:A:829:ASN:HB3	1:A:832:ARG:HA	1.94	0.50
1:A:436:ARG:HH12	1:A:571:THR:HB	1.77	0.50
1:A:78:ARG:HB3	1:A:86:LEU:HB3	1.93	0.49
2:B:288:ASP:OD1	2:B:289:TYR:N	2.37	0.49
2:B:243:SER:OG	2:B:352:ARG:NH2	2.44	0.49
3:C:1420:PRO:HG2	3:C:1503:ILE:HG13	1.95	0.49
1:A:253:VAL:HB	1:A:267:PHE:HB2	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:PRO:HA	1:A:358:ILE:HG13	1.93	0.49
1:A:449:VAL:O	1:A:449:VAL:HG12	2.13	0.49
1:A:820:MET:HG3	1:A:886:VAL:HG22	1.95	0.49
1:A:952:THR:OG1	1:A:953:TRP:N	2.46	0.49
2:B:295:MET:O	2:B:299:LEU:HB2	2.13	0.49
2:B:318:TYR:HA	2:B:321:TYR:HB2	1.95	0.49
1:A:498:LEU:HD23	1:A:558:PHE:HD2	1.77	0.49
1:A:299:LEU:HD21	2:B:257:ALA:HB3	1.95	0.49
1:A:402:PRO:HB3	1:A:429:VAL:HG13	1.94	0.48
1:A:104:LYS:HD3	1:A:132:ASP:HB2	1.95	0.48
1:A:489:ARG:H	1:A:489:ARG:HD3	1.79	0.48
1:A:139:TYR:OH	1:A:186:ASP:OD2	2.28	0.48
1:A:444:ASN:HB3	1:A:480:LYS:HB3	1.96	0.48
2:B:12:SER:OG	2:B:13:CYS:N	2.46	0.48
1:A:77:ASN:HB3	1:A:87:GLU:HG3	1.96	0.48
1:A:81:ALA:HB3	1:A:84:ASP:HB2	1.96	0.47
1:A:124:PRO:HB2	1:A:156:GLN:HG2	1.95	0.47
2:B:608:CYS:O	2:B:612:LYS:N	2.37	0.47
1:A:795:LEU:HB3	1:A:884:CYS:HB2	1.96	0.47
2:B:244:HIS:HB2	2:B:304:ILE:HA	1.96	0.47
1:A:347:LEU:HA	1:A:410:GLY:HA3	1.95	0.47
1:A:819:PRO:HD3	1:A:893:LYS:HE3	1.96	0.47
2:B:133:ASN:HB3	2:B:137:LYS:HG3	1.97	0.47
2:B:162:SER:O	2:B:164:TYR:N	2.47	0.47
1:A:783:ARG:HG3	1:A:894:SER:HB3	1.97	0.47
2:B:160:PRO:C	2:B:161:VAL:CG1	2.82	0.47
2:B:375:LEU:HD21	2:B:630:THR:HG22	1.96	0.47
1:A:666:LEU:HD11	1:A:693:LEU:HD13	1.97	0.47
2:B:673:SER:O	2:B:674:SER:OG	2.29	0.47
1:A:114:TRP:O	1:A:115:ARG:HB3	2.15	0.46
1:A:494:GLN:HB2	1:A:562:ARG:HB3	1.96	0.46
1:A:602:CYS:HA	1:A:636:GLU:OE2	2.15	0.46
2:B:239:ARG:O	2:B:244:HIS:NE2	2.48	0.46
2:B:365:GLU:HG2	2:B:407:PRO:HD3	1.96	0.46
2:B:375:LEU:HD22	2:B:633:ARG:HG2	1.97	0.46
1:A:543:ARG:NH1	1:A:547:GLU:OE1	2.47	0.46
1:A:405:GLY:C	1:A:407:SER:H	2.19	0.46
2:B:339:ASN:CG	2:B:340:VAL:N	2.69	0.46
1:A:93:TRP:CD1	1:A:111:LEU:HD22	2.50	0.46
2:B:480:PRO:C	2:B:482:GLN:H	2.19	0.46
1:A:745:ARG:NH2	2:B:591:PRO:HB2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:797:LEU:HD23	1:A:882:ILE:HD12	1.98	0.46
2:B:21:PRO:O	2:B:93:ARG:NH1	2.49	0.46
1:A:295:ILE:HB	1:A:316:SER:HB3	1.98	0.45
1:A:114:TRP:CE3	1:A:116:THR:HG22	2.51	0.45
1:A:284:ASP:OD1	1:A:289:ASP:N	2.47	0.45
1:A:3:LEU:HG	1:A:350:LEU:HD21	1.98	0.45
2:B:311:THR:O	2:B:315:VAL:HG23	2.17	0.45
2:B:249:THR:HG22	2:B:309:ALA:HB3	1.98	0.45
1:A:339:ARG:HD2	1:A:364:TYR:CD1	2.51	0.45
2:B:517:THR:OG1	2:B:518:GLY:N	2.49	0.45
2:B:66:ASP:HB3	2:B:85:PRO:HB3	1.98	0.45
3:C:1503:ILE:HG22	3:C:1504:SER:H	1.81	0.45
2:B:151:ILE:O	2:B:196:LEU:HA	2.16	0.45
1:A:797:LEU:HB3	1:A:882:ILE:HB	1.98	0.45
5:A:1011:BMA:H3	6:A:1012:MAN:H5	1.99	0.45
1:A:404:PHE:HE1	1:A:433:ILE:HD12	1.80	0.45
1:A:528:SER:OG	1:A:529:ARG:N	2.49	0.45
3:C:1420:PRO:O	3:C:1421:ARG:HB3	2.17	0.45
1:A:232:ASN:N	1:A:232:ASN:OD1	2.48	0.44
1:A:638:ALA:HA	1:A:721:ASN:HD21	1.81	0.44
1:A:804:ASN:O	1:A:806:ASN:ND2	2.49	0.44
2:B:561:THR:HG22	2:B:563:ARG:H	1.82	0.44
2:B:50:ALA:N	2:B:51:PRO:HD3	2.32	0.44
3:C:1486:THR:HG22	3:C:1503:ILE:O	2.17	0.44
2:B:21:PRO:HB3	2:B:96:ASP:HB2	2.00	0.44
2:B:5:CYS:HB3	2:B:38:CYS:O	2.17	0.44
1:A:510:ARG:HG2	1:A:548:PHE:CD1	2.53	0.44
1:A:548:PHE:CE1	1:A:550:ASP:HA	2.52	0.44
2:B:619:LYS:HD3	2:B:619:LYS:HA	1.81	0.44
2:B:172:ALA:HA	2:B:175:ASN:O	2.17	0.44
4:A:1005:NAG:H83	4:A:1005:NAG:O4	2.18	0.44
1:A:301:MET:HG2	1:A:311:GLU:HB2	1.99	0.44
2:B:102:ILE:HG23	2:B:397:PHE:HB2	1.99	0.44
2:B:441:ALA:HB1	2:B:455:PHE:HE1	1.83	0.44
1:A:139:TYR:CZ	1:A:141:PRO:HG3	2.53	0.43
2:B:128:LEU:O	2:B:131:ILE:HG22	2.18	0.43
2:B:169:PRO:HA	2:B:170:PRO:HD3	1.84	0.43
5:A:1009:BMA:H62	5:A:1011:BMA:H2	1.48	0.43
2:B:160:PRO:O	2:B:161:VAL:CG1	2.66	0.43
2:B:569:SER:OG	2:B:570:SER:N	2.51	0.43
1:A:551:LYS:HA	1:A:551:LYS:HD3	1.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:ARG:CZ	4:B:702:NAG:H2	2.48	0.43
3:C:1485:ILE:HG22	3:C:1486:THR:H	1.84	0.43
1:A:869:ILE:HD11	1:A:919:SER:HB3	1.98	0.43
2:B:267:GLN:HA	2:B:268:PRO:HD3	1.88	0.43
2:B:671:GLU:HG3	2:B:672:ASP:H	1.83	0.43
1:A:114:TRP:CD2	1:A:116:THR:HA	2.53	0.43
2:B:105:ARG:NE	2:B:394:THR:OG1	2.46	0.43
4:B:705:NAG:O4	4:B:706:NAG:H61	2.18	0.43
1:A:510:ARG:HH12	1:A:553:THR:HB	1.84	0.43
1:A:68:GLN:HA	1:A:69:PRO:HD3	1.88	0.42
2:B:164:TYR:CE1	2:B:263:ALA:HB2	2.54	0.42
2:B:473:CYS:SG	2:B:474:SER:N	2.85	0.42
1:A:869:ILE:HA	1:A:917:SER:HB2	2.01	0.42
1:A:315:VAL:HG21	1:A:360:ILE:HD13	2.00	0.42
2:B:589:ILE:HG13	2:B:589:ILE:H	1.71	0.42
1:A:419:TYR:CE1	1:A:439:PRO:HA	2.54	0.42
1:A:605:LYS:H	1:A:635:GLY:HA3	1.84	0.42
3:C:1421:ARG:CB	3:C:1503:ILE:HD12	2.46	0.42
1:A:26:PHE:HB2	1:A:37:LEU:HG	2.02	0.42
1:A:514:LEU:HA	1:A:541:TYR:CD1	2.55	0.42
1:A:724:ASP:N	1:A:724:ASP:OD2	2.52	0.42
1:A:790:PHE:CZ	1:A:889:LEU:HB2	2.55	0.42
1:A:809:LEU:HG	1:A:920:LEU:HD13	2.01	0.42
2:B:86:GLN:O	2:B:425:LEU:HD12	2.19	0.42
1:A:529:ARG:HG2	1:A:530:GLY:H	1.83	0.42
2:B:308:PHE:HB2	2:B:330:VAL:HG22	2.01	0.42
3:C:1420:PRO:HB2	3:C:1421:ARG:H	1.54	0.42
2:B:524:ASP:OD1	2:B:525:ASP:N	2.53	0.42
1:A:651:ALA:O	1:A:677:ARG:NH1	2.38	0.42
1:A:647:ILE:HG22	1:A:713:PHE:CE2	2.54	0.42
2:B:160:PRO:O	2:B:161:VAL:HG12	2.20	0.42
3:C:1447:TYR:HB2	3:C:1465:VAL:HG23	2.02	0.42
1:A:178:TYR:CE1	3:C:1493:ARG:HB3	2.55	0.42
1:A:514:LEU:HA	1:A:541:TYR:HD1	1.85	0.42
2:B:240:ASN:N	2:B:240:ASN:OD1	2.51	0.41
2:B:456:GLU:HB3	2:B:459:VAL:HB	2.02	0.41
2:B:191:LYS:HE2	2:B:280:HIS:NE2	2.35	0.41
2:B:5:CYS:SG	2:B:40:LEU:HD23	2.60	0.41
1:A:438:ARG:O	1:A:440:VAL:HG23	2.20	0.41
2:B:320:ASN:ND2	4:B:702:NAG:O7	2.47	0.41
1:A:376:PHE:HB3	1:A:383:LEU:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:527:ILE:HG22	1:A:528:SER:H	1.86	0.41
1:A:65:ARG:HA	1:A:65:ARG:HD3	1.92	0.41
2:B:445:SER:O	2:B:446:HIS:HB2	2.21	0.41
3:C:1427:ALA:H	3:C:1434:LEU:HB3	1.86	0.41
2:B:362:LEU:HD12	2:B:363:PRO:HD2	2.02	0.41
2:B:79:GLN:HB2	2:B:80:VAL:H	1.73	0.41
1:A:111:LEU:O	1:A:113:HIS:ND1	2.54	0.41
1:A:335:GLU:OE2	1:A:366:GLY:N	2.53	0.41
2:B:223:PHE:HB3	2:B:290:PRO:HG2	2.02	0.41
2:B:516:ILE:HG12	2:B:526:PHE:HE2	1.86	0.41
1:A:2:ASN:ND2	1:A:350:LEU:O	2.53	0.41
1:A:24:ASP:HA	1:A:409:LYS:HG2	2.03	0.41
2:B:230:THR:HG23	2:B:304:ILE:HD12	2.02	0.41
2:B:334:SER:O	2:B:339:ASN:HB2	2.21	0.41
2:B:672:ASP:N	2:B:672:ASP:OD1	2.54	0.41
1:A:439:PRO:HD2	1:A:576:PRO:HA	2.03	0.40
2:B:139:ALA:O	2:B:142:MET:N	2.53	0.40
2:B:67:ARG:N	2:B:86:GLN:OE1	2.45	0.40
1:A:174:PRO:HB2	2:B:262:LEU:HD21	2.02	0.40
2:B:476:GLU:C	2:B:478:TYR:H	2.24	0.40
3:C:1421:ARG:CG	3:C:1422:ASP:N	2.72	0.40
1:A:272:MET:SD	2:B:320:ASN:HB3	2.61	0.40
1:A:645:VAL:HG22	1:A:715:LEU:HD22	2.03	0.40
2:B:297:GLU:O	2:B:301:GLN:HG2	2.22	0.40
1:A:749:SER:HA	1:A:750:PRO:HA	1.85	0.40
3:C:1471:THR:OG1	3:C:1472:ALA:N	2.55	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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	920/959 (96%)	847 (92%)	69 (8%)	4 (0%)	36	70
2	B	688/692 (99%)	597 (87%)	85 (12%)	6 (1%)	19	54
3	C	91/98 (93%)	73 (80%)	16 (18%)	2 (2%)	7	35
All	All	1699/1749 (97%)	1517 (89%)	170 (10%)	12 (1%)	24	59

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	451	PRO
2	B	162	SER
2	B	163	PRO
1	A	833	ILE
2	B	161	VAL
2	B	164	TYR
3	C	1420	PRO
1	A	452	SER
3	C	1421	ARG
2	B	48	ASN
2	B	78	SER
1	A	440	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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	784/813 (96%)	748 (95%)	36 (5%)	29	64
2	B	612/614 (100%)	580 (95%)	32 (5%)	25	60
3	C	78/81 (96%)	69 (88%)	9 (12%)	6	25
All	All	1474/1508 (98%)	1397 (95%)	77 (5%)	25	60

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ASP

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Mol	Chain	Res	Type
1	A	58	LYS
1	A	79	ASP
1	A	115	ARG
1	A	134	THR
1	A	249	THR
1	A	260	ASN
1	A	261	MET
1	A	275	TYR
1	A	283	THR
1	A	299	LEU
1	A	321	ARG
1	A	331	LEU
1	A	430	ASP
1	A	452	SER
1	A	453	ILE
1	A	454	LEU
1	A	461	CYS
1	A	463	LEU
1	A	474	ASN
1	A	489	ARG
1	A	532	LEU
1	A	548	PHE
1	A	551	LYS
1	A	567	THR
1	A	650	GLN
1	A	674	ASN
1	A	724	ASP
1	A	729	VAL
1	A	757	ILE
1	A	768	THR
1	A	806	ASN
1	A	817	ASP
1	A	833	ILE
1	A	916	HIS
1	A	933	TYR
2	B	26	CYS
2	B	44	LEU
2	B	47	ASP
2	B	71	ASP
2	B	80	VAL
2	B	90	LEU
2	B	116	TYR

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Mol	Chain	Res	Type
2	B	138	LEU
2	B	149	LEU
2	B	165	MET
2	B	207	VAL
2	B	215	ASN
2	B	216	ARG
2	B	217	ASP
2	B	220	GLU
2	B	224	ASP
2	B	311	THR
2	B	342	GLN
2	B	344	ILE
2	B	371	ASN
2	B	454	THR
2	B	462	CYS
2	B	466	TRP
2	B	478	TYR
2	B	494	VAL
2	B	506	CYS
2	B	509	HIS
2	B	521	CYS
2	B	528	CYS
2	B	589	ILE
2	B	608	CYS
2	B	647	ASP
3	C	1419	VAL
3	C	1423	LEU
3	C	1463	PHE
3	C	1469	LYS
3	C	1483	TYR
3	C	1484	THR
3	C	1487	VAL
3	C	1493	ARG
3	C	1503	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	509	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 41 ligands modelled in this entry, 8 are monoatomic - leaving 33 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$
4	NAG	A	1001	1,4	14,14,15	0.46	0	17,19,21	0.47	0
4	NAG	A	1002	5,4	14,14,15	0.23	0	17,19,21	0.46	0
5	BMA	A	1003	4,6	11,11,12	0.90	0	15,15,17	1.12	1 (6%)
6	MAN	A	1004	5	11,11,12	0.68	0	15,15,17	1.08	2 (13%)
4	NAG	A	1005	1,4	14,14,15	1.03	1 (7%)	17,19,21	1.67	4 (23%)
4	NAG	A	1006	4	14,14,15	0.24	0	17,19,21	0.41	0
4	NAG	A	1007	1,4	14,14,15	0.33	0	17,19,21	0.45	0
4	NAG	A	1008	5,4	14,14,15	0.24	0	17,19,21	0.44	0
5	BMA	A	1009	5,4,6	11,11,12	0.69	0	15,15,17	0.80	0
6	MAN	A	1010	5	11,11,12	0.71	0	15,15,17	1.04	2 (13%)
5	BMA	A	1011	5,6	11,11,12	1.19	2 (18%)	15,15,17	1.12	1 (6%)
6	MAN	A	1012	5	11,11,12	1.02	1 (9%)	15,15,17	1.66	4 (26%)
4	NAG	A	1013	1,4	14,14,15	0.23	0	17,19,21	0.46	0
4	NAG	A	1014	5,4	14,14,15	0.28	0	17,19,21	0.42	0
5	BMA	A	1015	4,6	11,11,12	0.65	0	15,15,17	0.74	0
6	MAN	A	1016	5	11,11,12	0.66	0	15,15,17	1.03	2 (13%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	A	1017	1	14,14,15	0.23	0	17,19,21	0.45	0
4	NAG	A	1018	1,4	14,14,15	0.21	0	17,19,21	0.46	0
4	NAG	A	1019	4	14,14,15	0.24	0	17,19,21	0.42	0
4	NAG	A	1020	1	14,14,15	0.72	1 (7%)	17,19,21	0.95	1 (5%)
4	NAG	A	1021	1	14,14,15	0.21	0	17,19,21	0.49	0
4	NAG	A	1022	1,4	14,14,15	0.26	0	17,19,21	0.45	0
4	NAG	A	1023	4	14,14,15	0.46	0	17,19,21	0.68	1 (5%)
4	NAG	A	1024	1,4	14,14,15	0.28	0	17,19,21	0.46	0
4	NAG	A	1025	5,4	14,14,15	0.32	0	17,19,21	0.55	0
5	BMA	A	1026	4	11,11,12	0.95	1 (9%)	15,15,17	1.49	3 (20%)
4	NAG	B	701	2	14,14,15	0.72	1 (7%)	17,19,21	0.98	1 (5%)
4	NAG	B	702	2	14,14,15	0.32	0	17,19,21	0.57	0
4	NAG	B	703	2,4	14,14,15	0.45	0	17,19,21	0.93	1 (5%)
4	NAG	B	704	4	14,14,15	0.23	0	17,19,21	1.01	1 (5%)
4	NAG	B	705	2,4	14,14,15	0.26	0	17,19,21	0.45	0
4	NAG	B	706	5,4	14,14,15	0.73	1 (7%)	17,19,21	0.98	1 (5%)
5	BMA	B	707	4	11,11,12	0.79	0	15,15,17	1.19	2 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1001	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1002	5,4	-	0/6/23/26	0/1/1/1
5	BMA	A	1003	4,6	-	0/2/19/22	0/1/1/1
6	MAN	A	1004	5	-	0/2/19/22	0/1/1/1
4	NAG	A	1005	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1006	4	-	0/6/23/26	0/1/1/1
4	NAG	A	1007	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1008	5,4	-	0/6/23/26	0/1/1/1
5	BMA	A	1009	5,4,6	-	0/2/19/22	0/1/1/1
6	MAN	A	1010	5	-	0/2/19/22	0/1/1/1
5	BMA	A	1011	5,6	-	0/2/19/22	0/1/1/1
6	MAN	A	1012	5	-	0/2/19/22	0/1/1/1
4	NAG	A	1013	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1014	5,4	-	0/6/23/26	0/1/1/1
5	BMA	A	1015	4,6	-	0/2/19/22	0/1/1/1
6	MAN	A	1016	5	-	0/2/19/22	0/1/1/1
4	NAG	A	1017	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1018	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1019	4	-	0/6/23/26	0/1/1/1
4	NAG	A	1020	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1021	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1022	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1023	4	-	0/6/23/26	0/1/1/1
4	NAG	A	1024	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1025	5,4	-	0/6/23/26	0/1/1/1
5	BMA	A	1026	4	-	0/2/19/22	0/1/1/1
4	NAG	B	701	2	-	0/6/23/26	0/1/1/1
4	NAG	B	702	2	-	0/6/23/26	0/1/1/1
4	NAG	B	703	2,4	-	0/6/23/26	0/1/1/1
4	NAG	B	704	4	-	0/6/23/26	0/1/1/1
4	NAG	B	705	2,4	-	0/6/23/26	0/1/1/1
4	NAG	B	706	5,4	-	0/6/23/26	0/1/1/1
5	BMA	B	707	4	-	0/2/19/22	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1005	NAG	O5-C1	-3.61	1.37	1.43
5	A	1011	BMA	O5-C5	2.07	1.47	1.43
5	A	1011	BMA	C4-C5	2.24	1.57	1.53
5	A	1026	BMA	C1-C2	2.36	1.57	1.52
4	A	1020	NAG	O5-C1	2.47	1.47	1.43
4	B	701	NAG	O5-C1	2.55	1.47	1.43
4	B	706	NAG	O5-C1	2.55	1.47	1.43
6	A	1012	MAN	C1-C2	2.70	1.58	1.52

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1016	MAN	O2-C2-C3	-2.37	105.57	110.19
6	A	1010	MAN	O2-C2-C3	-2.36	105.59	110.19
6	A	1012	MAN	O2-C2-C3	-2.36	105.59	110.19
6	A	1004	MAN	O2-C2-C3	-2.28	105.74	110.19
4	A	1005	NAG	C4-C3-C2	2.02	113.98	111.02
5	B	707	BMA	O5-C1-C2	2.03	113.94	110.78
6	A	1010	MAN	C1-O5-C5	2.10	115.07	112.19
6	A	1016	MAN	C1-O5-C5	2.24	115.27	112.19
4	A	1023	NAG	C1-O5-C5	2.38	115.46	112.19
5	A	1026	BMA	C1-O5-C5	2.50	115.63	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1005	NAG	C1-C2-N2	2.55	114.84	110.49
5	A	1026	BMA	C1-C2-C3	2.66	113.02	109.66
5	B	707	BMA	C1-O5-C5	2.70	115.90	112.19
4	B	703	NAG	C1-O5-C5	2.73	115.95	112.19
6	A	1004	MAN	C1-O5-C5	2.74	115.95	112.19
5	A	1011	BMA	C1-O5-C5	2.75	115.97	112.19
5	A	1026	BMA	O5-C1-C2	2.80	115.15	110.78
5	A	1003	BMA	O3-C3-C2	2.84	115.32	110.04
6	A	1012	MAN	C1-C2-C3	3.10	113.58	109.66
4	A	1005	NAG	C3-C4-C5	3.13	115.84	110.24
6	A	1012	MAN	O5-C1-C2	3.15	115.68	110.78
6	A	1012	MAN	C1-O5-C5	3.23	116.63	112.19
4	B	704	NAG	C1-O5-C5	3.48	116.98	112.19
4	B	706	NAG	C1-O5-C5	3.58	117.11	112.19
4	A	1020	NAG	C1-O5-C5	3.60	117.14	112.19
4	B	701	NAG	C1-O5-C5	3.70	117.28	112.19
4	A	1005	NAG	C2-N2-C7	4.50	129.51	122.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1005	NAG	1	0
5	A	1009	BMA	1	0
5	A	1011	BMA	2	0
6	A	1012	MAN	1	0
5	A	1015	BMA	2	0
4	A	1020	NAG	2	0
4	B	702	NAG	2	0
4	B	703	NAG	1	0
4	B	705	NAG	1	0
4	B	706	NAG	1	0

## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	924/959 (96%)	-0.07	12 (1%)	77 77	42, 87, 140, 175	0
2	B	690/692 (99%)	0.16	31 (4%)	33 33	49, 102, 207, 251	1 (0%)
3	C	93/98 (94%)	2.18	40 (43%)	0 0	74, 188, 325, 345	0
All	All	1707/1749 (97%)	0.14	83 (4%)	29 29	42, 95, 198, 345	1 (0%)

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	1428	ALA	11.3
2	B	674	SER	8.8
2	B	443	PRO	8.6
3	C	1426	VAL	7.1
3	C	1417	SER	7.1
2	B	460	CYS	6.6
3	C	1427	ALA	5.9
2	B	444	ASN	5.7
3	C	1507	TYR	5.5
3	C	1505	ILE	5.4
3	C	1460	VAL	5.3
3	C	1429	THR	5.2
3	C	1433	LEU	5.2
2	B	509	HIS	5.1
3	C	1432	SER	4.9
3	C	1476	GLY	4.7
3	C	1430	PRO	4.5
3	C	1451	TYR	4.4
2	B	442	GLU	4.4
3	C	1425	VAL	4.3
2	B	1	GLY	4.3
2	B	459	VAL	4.3
3	C	1452	GLY	4.2

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Mol	Chain	Res	Type	RSRZ
3	C	1474	ILE	4.1
2	B	35	SER	4.1
3	C	1461	GLN	4.1
3	C	1509	THR	4.0
3	C	1481	VAL	4.0
2	B	677	SER	3.9
2	B	644	GLU	3.7
3	C	1449	ILE	3.7
2	B	461	ARG	3.7
3	C	1482	ASP	3.6
3	C	1487	VAL	3.6
2	B	510	SER	3.5
3	C	1475	SER	3.4
3	C	1508	ARG	3.4
3	C	1450	THR	3.3
3	C	1462	GLU	3.2
1	A	532	LEU	3.2
2	B	53	SER	3.2
2	B	37	ARG	3.2
2	B	464	PRO	3.1
3	C	1506	ASN	3.1
2	B	456	GLU	3.1
2	B	36	PRO	3.0
2	B	52	GLU	2.9
3	C	1421	ARG	2.9
3	C	1478	LYS	2.8
3	C	1483	TYR	2.7
1	A	461	CYS	2.7
3	C	1459	PRO	2.7
1	A	509	ARG	2.7
1	A	531	GLY	2.7
2	B	441	ALA	2.6
3	C	1435	ILE	2.6
1	A	493	PHE	2.6
2	B	515	LYS	2.6
2	B	2	PRO	2.5
1	A	491	LEU	2.5
2	B	449	ASN	2.5
2	B	472	GLU	2.5
1	A	506	GLY	2.4
3	C	1457	ASN	2.4
3	C	1485	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	670	PHE	2.3
2	B	481	SER	2.3
1	A	906	GLU	2.3
3	C	1418	ASP	2.3
3	C	1473	THR	2.2
3	C	1484	THR	2.2
3	C	1436	SER	2.2
2	B	337	SER	2.2
3	C	1423	LEU	2.2
2	B	34	GLY	2.2
3	C	1504	SER	2.2
1	A	918	TYR	2.1
2	B	673	SER	2.1
1	A	441	ILE	2.1
2	B	478	TYR	2.1
1	A	550	ASP	2.1
2	B	678	ILE	2.1
2	B	455	PHE	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	BMA	A	1026	11/12	0.52	0.41	175,181,190,190	0
4	NAG	A	1020	14/15	0.70	0.36	136,151,158,158	0
4	NAG	A	1025	14/15	0.71	0.41	129,145,164,177	0
5	BMA	A	1003	11/12	0.73	0.39	148,158,162,169	0
6	MAN	A	1010	11/12	0.75	0.21	114,126,140,141	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	A	1014	14/15	0.76	0.29	123,139,153,160	0
6	MAN	A	1016	11/12	0.76	0.25	161,170,176,179	0
6	MAN	A	1004	11/12	0.77	0.47	164,172,177,180	0
4	NAG	A	1023	14/15	0.78	0.37	141,148,157,159	0
5	BMA	B	707	11/12	0.81	0.15	100,109,116,117	0
4	NAG	A	1006	14/15	0.81	0.34	125,134,144,148	0
5	BMA	A	1015	11/12	0.83	0.43	156,158,170,178	0
4	NAG	A	1017	14/15	0.83	0.25	124,142,149,152	0
4	NAG	B	704	14/15	0.83	0.24	140,144,159,165	0
4	NAG	A	1019	14/15	0.86	0.18	123,132,135,138	0
4	NAG	A	1021	14/15	0.87	0.22	92,108,117,120	0
4	NAG	B	701	14/15	0.88	0.27	99,127,136,146	0
4	NAG	A	1022	14/15	0.88	0.21	97,118,133,136	0
4	NAG	B	703	14/15	0.89	0.20	91,117,137,142	0
5	BMA	A	1011	11/12	0.90	0.13	92,107,128,129	0
4	NAG	A	1013	14/15	0.91	0.20	92,110,124,132	0
4	NAG	B	702	14/15	0.91	0.17	80,95,106,114	0
4	NAG	A	1002	14/15	0.91	0.22	103,115,120,138	0
4	NAG	B	706	14/15	0.92	0.20	93,108,120,120	0
5	BMA	A	1009	11/12	0.93	0.09	93,100,116,127	0
7	MN	B	709	1/1	0.93	0.20	88,88,88,88	0
4	NAG	A	1018	14/15	0.93	0.14	101,117,128,132	0
6	MAN	A	1012	11/12	0.94	0.18	103,110,119,120	0
4	NAG	A	1001	14/15	0.95	0.17	66,76,92,96	0
4	NAG	A	1024	14/15	0.95	0.13	64,88,106,108	0
4	NAG	A	1008	14/15	0.95	0.14	44,60,84,91	0
7	MN	A	1029	1/1	0.95	0.14	177,177,177,177	0
7	MN	A	1030	1/1	0.96	0.16	137,137,137,137	0
4	NAG	A	1005	14/15	0.96	0.26	96,114,123,131	0
4	NAG	A	1007	14/15	0.97	0.13	40,54,83,85	0
4	NAG	B	705	14/15	0.97	0.14	61,87,93,93	0
7	MN	A	1031	1/1	0.98	0.10	84,84,84,84	0
7	MN	B	708	1/1	0.99	0.17	48,48,48,48	0
7	MN	B	710	1/1	0.99	0.23	56,56,56,56	0
7	MN	A	1028	1/1	0.99	0.12	90,90,90,90	0
7	MN	A	1027	1/1	1.00	0.07	89,89,89,89	0

## 6.5 Other polymers

There are no such residues in this entry.