



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 03:12 PM BST

PDB ID : 6EA7  
Title : Structure of EBOV GPcl in complex with the pan-ebolavirus mAb ADI-15878  
Authors : West, B.R.; Moyer, C.L.; King, L.B.; Fusco, M.L.; Milligan, J.C.; Hui, S.;  
Saphire, E.O.  
Deposited on : 2018-08-02  
Resolution : 4.25 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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

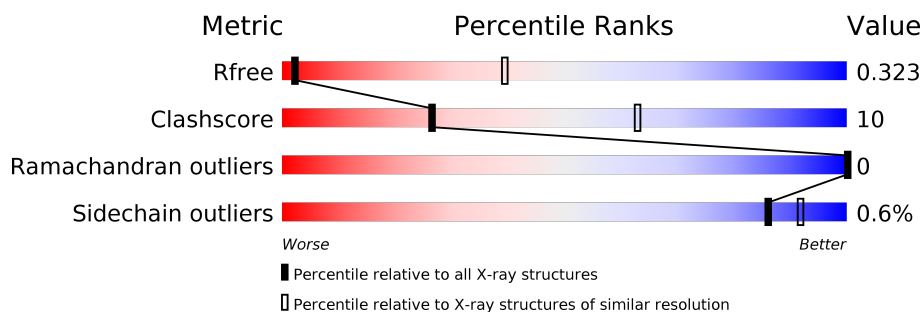
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.25 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))
$R_{free}$	130704	1017 (4.72-3.78)
Clashscore	141614	1059 (4.72-3.80)
Ramachandran outliers	138981	1014 (4.72-3.80)
Sidechain outliers	138945	1018 (4.72-3.78)

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 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	163	75% 25%
1	C	163	75% 23% .
1	E	163	77% 19% .
2	B	111	73% 23% 5%
2	D	111	76% 18% 6%
2	F	111	77% 16% 7%
3	H	233	73% 18% 9%

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Mol	Chain	Length	Quality of chain
3	M	233	 70%23%7%
3	Q	233	 73%21%• 5%
4	L	213	 80%18%•
4	N	213	 80%19%•
4	R	213	 78%20%••
5	G	3	 67%33%
6	I	8	 38%63%
6	J	8	 25%63%13%
7	K	7	 57%14%29%

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 16154 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 Envelope glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	163	Total	C	N	O	S	0	0	0
			1252	798	218	231	5			
1	C	159	Total	C	N	O	S	0	0	0
			1213	770	213	225	5			
1	E	156	Total	C	N	O	S	0	0	0
			1190	756	208	221	5			

- Molecule 2 is a protein called Envelope glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	106	Total	C	N	O	S	0	0	0
			830	530	144	150	6			
2	D	104	Total	C	N	O	S	0	0	0
			816	522	141	147	6			
2	F	103	Total	C	N	O	S	0	0	0
			809	517	140	146	6			

- Molecule 3 is a protein called ADI-15878 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	213	Total	C	N	O	S	0	0	0
			1598	1016	269	307	6			
3	M	217	Total	C	N	O	S	0	0	0
			1625	1031	274	314	6			
3	Q	222	Total	C	N	O	S	0	0	0
			1655	1047	280	322	6			

- Molecule 4 is a protein called ADI-15878 Fab Light Chain.

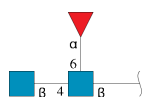
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	210	Total	C	N	O	S	0	0	0
			1597	999	261	333	4			

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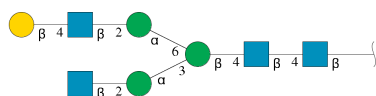
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	N	211	Total	C	N	O	S	0	0	0
			1606	1005	263	334	4			
4	R	211	Total	C	N	O	S	0	0	0
			1608	1006	266	332	4			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



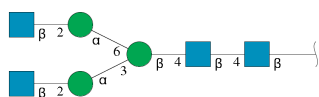
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	G	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 6 is an oligosaccharide called beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



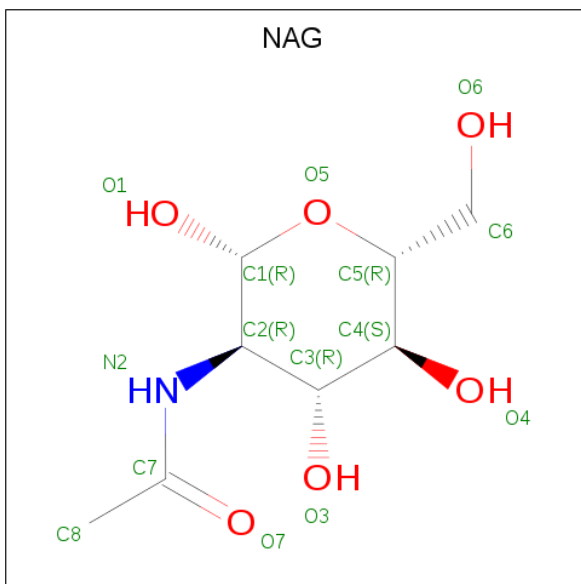
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	I	8	Total	C	N	O	0	0	0
			100	56	4	40			
6	J	8	Total	C	N	O	0	0	0
			100	56	4	40			

- Molecule 7 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	K	7	Total	C	N	O	0	0	0
			89	50	4	35			

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).

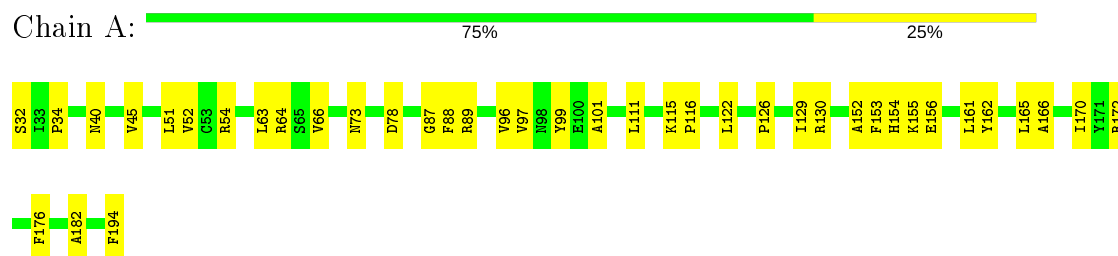


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	C	1	Total	C	N	O	0	0
			14	8	1	5		
8	E	1	Total	C	N	O	0	0
			14	8	1	5		

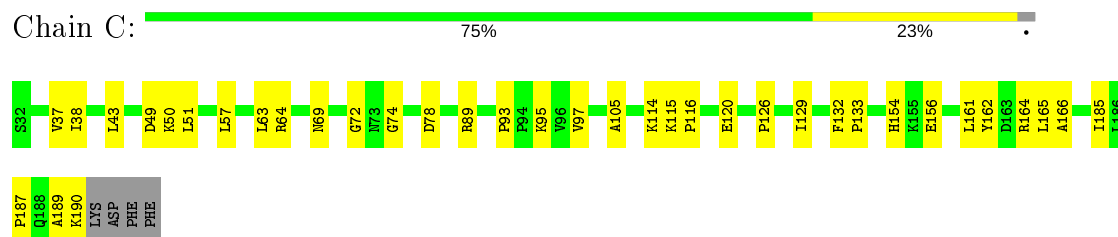
### 3 Residue-property plots [i](#)

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.

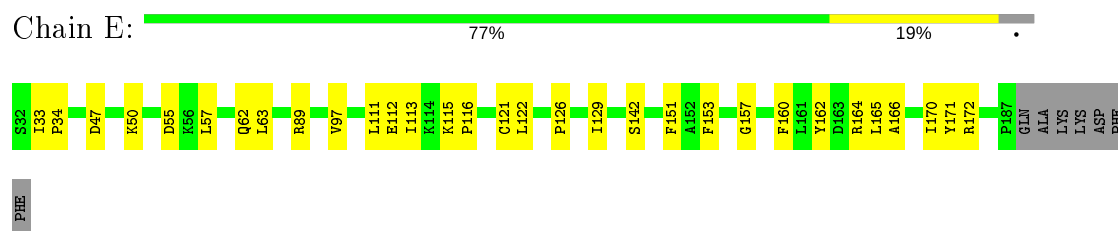
- Molecule 1: Envelope glycoprotein



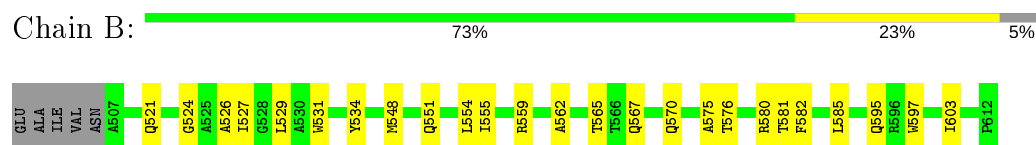
- Molecule 1: Envelope glycoprotein



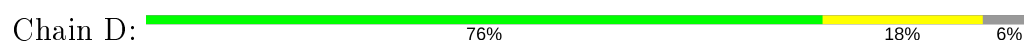
- Molecule 1: Envelope glycoprotein



- Molecule 2: Envelope glycoprotein



- Molecule 2: Envelope glycoprotein

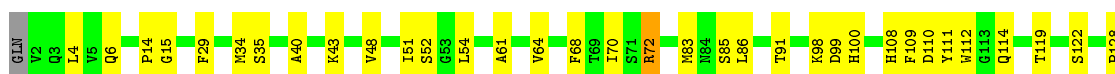




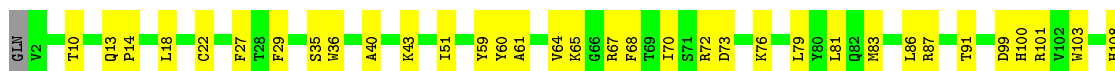
- Molecule 2: Envelope glycoprotein



- Molecule 3: ADI-15878 Fab Heavy Chain



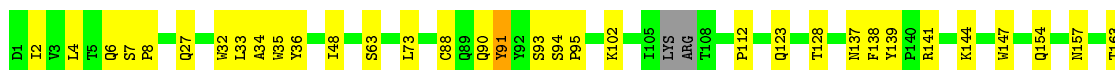
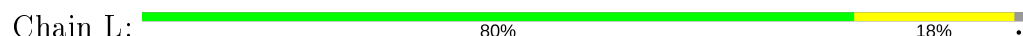
- Molecule 3: ADI-15878 Fab Heavy Chain



- Molecule 3: ADI-15878 Fab Heavy Chain

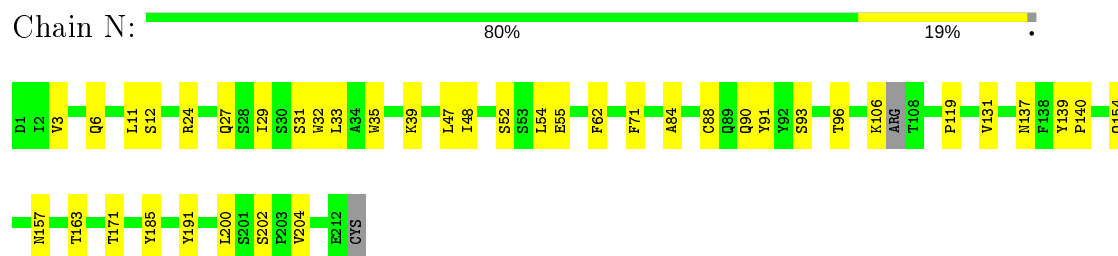


- Molecule 4: ADI-15878 Fab Light Chain

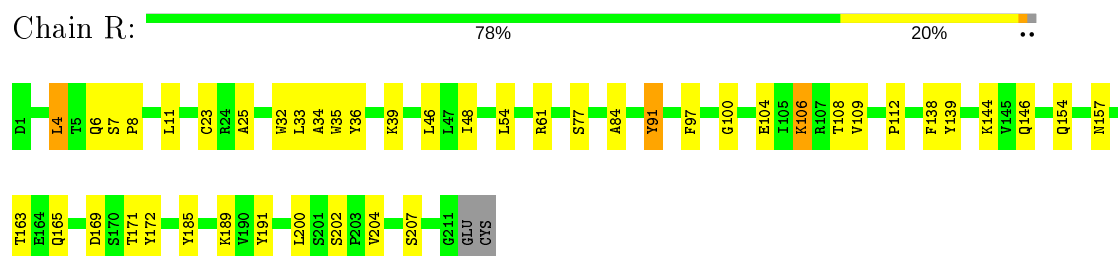




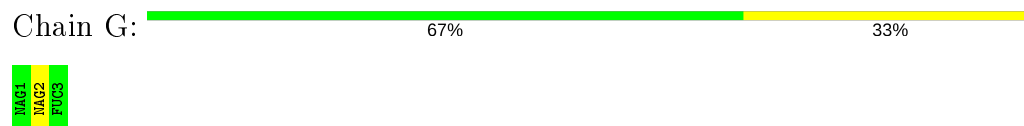
- Molecule 4: ADI-15878 Fab Light Chain



- Molecule 4: ADI-15878 Fab Light Chain



- Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



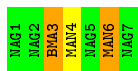
- Molecule 6: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyra

nose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K: 57% 14% 29%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	152.78Å 152.78Å 247.69Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	56.08 – 4.25 90.42 – 4.25	Depositor EDS
% Data completeness (in resolution range)	99.9 (56.08-4.25) 100.0 (90.42-4.25)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.39 (at 4.30Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, $R_{free}$	0.280 , 0.324 0.281 , 0.323	Depositor DCC
$R_{free}$ test set	2013 reflections (8.33%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	133.2	Xtriage
Anisotropy	0.504	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , 71.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.31$ , $\langle L^2 \rangle = 0.14$	Xtriage
Estimated twinning fraction	0.206 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.71	EDS
Total number of atoms	16154	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	173.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.22% 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: FUC, GAL, NAG, BMA, 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	0.26	0/1283	0.47	0/1740
1	C	0.26	0/1242	0.47	0/1686
1	E	0.26	0/1219	0.47	0/1656
2	B	0.26	0/851	0.45	0/1159
2	D	0.25	0/837	0.44	0/1139
2	F	0.25	0/829	0.43	0/1128
3	H	0.24	0/1639	0.47	0/2236
3	M	0.25	0/1666	0.47	0/2271
3	Q	0.26	0/1697	0.48	0/2314
4	L	0.26	0/1631	0.50	0/2218
4	N	0.26	0/1640	0.48	0/2229
4	R	0.26	0/1643	0.48	0/2234
All	All	0.26	0/16177	0.47	0/22010

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	1252	0	1229	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1213	0	1194	29	0
1	E	1190	0	1168	25	0
2	B	830	0	806	26	0
2	D	816	0	794	19	0
2	F	809	0	786	27	0
3	H	1598	0	1560	33	0
3	M	1625	0	1588	59	0
3	Q	1655	0	1618	33	0
4	L	1597	0	1537	32	0
4	N	1606	0	1550	33	0
4	R	1608	0	1558	34	0
5	G	38	0	34	3	0
6	I	100	0	85	2	0
6	J	100	0	85	4	0
7	K	89	0	76	1	0
8	C	14	0	13	1	0
8	E	14	0	13	0	0
All	All	16154	0	15694	327	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 10.

All (327) 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)
3:M:72:ARG:CG	3:M:79:LEU:HD13	1.62	1.28
3:M:72:ARG:CG	3:M:79:LEU:CD1	2.37	1.01
3:M:29:PHE:CE1	3:M:72:ARG:NH1	2.29	1.00
3:M:72:ARG:HG2	3:M:79:LEU:HD13	1.38	1.00
1:E:162:TYR:HB2	1:E:165:LEU:O	1.66	0.95
3:M:51:ILE:CG2	3:M:72:ARG:HD3	1.97	0.94
3:M:51:ILE:HG21	3:M:72:ARG:HD3	1.51	0.93
3:M:72:ARG:HG2	3:M:79:LEU:CD1	2.01	0.89
3:M:72:ARG:HG3	3:M:79:LEU:CD1	2.03	0.88
3:H:29:PHE:CE2	3:H:34:MET:SD	2.67	0.87
3:M:29:PHE:HE1	3:M:72:ARG:NH1	1.69	0.86
3:M:72:ARG:HG3	3:M:79:LEU:HD13	1.58	0.86
3:M:67:ARG:HH11	3:M:87:ARG:HD3	1.42	0.85
2:F:525:ALA:HB1	2:F:527:ILE:CD1	2.06	0.84
3:H:29:PHE:HE2	3:H:34:MET:SD	2.02	0.83
3:M:72:ARG:CD	3:M:79:LEU:HD13	2.08	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:526:ALA:HB1	3:M:59:TYR:HB3	1.64	0.79
2:B:529:LEU:HD23	4:N:91:TYR:HB2	1.66	0.78
2:F:527:ILE:HG12	4:L:94:SER:H	1.48	0.78
1:E:122:LEU:HB2	1:E:172:ARG:HG3	1.66	0.77
2:D:533:PRO:HB2	1:E:153:PHE:HB3	1.67	0.76
3:H:6:GLN:H	3:H:114:GLN:HE22	1.33	0.76
3:Q:128:PRO:HB3	3:Q:154:TYR:HB3	1.66	0.75
4:L:147:TRP:HE1	4:L:176:SER:HG	1.34	0.74
3:M:135:PRO:HD2	3:M:222:PRO:HB3	1.69	0.74
5:G:2:NAG:H82	5:G:2:NAG:C1	2.18	0.73
2:F:527:ILE:HG21	4:L:95:PRO:HD3	1.70	0.73
4:R:106:LYS:HD3	4:R:139:TYR:HD2	1.53	0.73
3:M:67:ARG:NH1	3:M:87:ARG:HD3	2.03	0.72
3:Q:52:SER:O	3:Q:72:ARG:NH1	2.23	0.71
4:L:4:LEU:HD21	4:L:90:GLN:OE1	1.91	0.70
4:N:106:LYS:HE3	4:N:139:TYR:HB2	1.74	0.69
4:N:24:ARG:NH2	4:R:207:SER:OG	2.26	0.69
1:A:45:VAL:HB	3:H:54:LEU:HD22	1.73	0.69
4:L:4:LEU:CD2	4:L:90:GLN:OE1	2.40	0.69
4:L:33:LEU:HD21	4:L:88:CYS:HB2	1.76	0.68
4:L:32:TRP:HB3	4:L:91:TYR:CE1	2.28	0.68
3:M:51:ILE:HG21	3:M:72:ARG:CD	2.23	0.68
4:L:144:LYS:HB3	4:L:196:THR:HB	1.76	0.68
4:L:6:GLN:NE2	4:L:88:CYS:SG	2.66	0.67
3:H:14:PRO:HD3	3:H:122:SER:HB2	1.77	0.66
4:R:6:GLN:OE1	4:R:100:GLY:N	2.29	0.66
1:A:32:SER:N	2:F:523:GLU:OE2	2.29	0.65
1:C:187:PRO:HB2	1:C:190:LYS:HE3	1.79	0.65
5:G:2:NAG:H83	5:G:2:NAG:H3	1.79	0.65
2:B:548:MET:HG3	2:B:555:ILE:HD11	1.79	0.65
1:E:47:ASP:HB3	1:E:50:LYS:HG2	1.78	0.65
3:M:51:ILE:HG23	3:M:72:ARG:HD3	1.79	0.64
1:E:126:PRO:HD2	1:E:129:ILE:HD12	1.80	0.64
4:L:102:LYS:NZ	4:L:141:ARG:NH2	2.46	0.64
4:R:108:THR:HG22	4:R:109:VAL:N	2.13	0.64
3:M:72:ARG:HD2	3:M:79:LEU:HD13	1.79	0.64
4:L:32:TRP:HB3	4:L:91:TYR:HE1	1.63	0.63
4:N:3:VAL:HA	4:N:96:THR:HG21	1.80	0.63
1:E:160:PHE:O	1:E:162:TYR:CD2	2.51	0.63
4:L:102:LYS:HZ2	4:L:141:ARG:HH22	1.44	0.63
3:Q:175:PHE:HA	4:R:163:THR:HG22	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:27:GLN:HG3	4:R:189:LYS:HZ3	1.64	0.63
4:L:35:TRP:HB2	4:L:48:ILE:HG22	1.81	0.62
3:M:29:PHE:HE1	3:M:72:ARG:CZ	2.11	0.62
3:M:128:PRO:HB3	3:M:154:TYR:HB3	1.80	0.62
3:M:51:ILE:CG2	3:M:72:ARG:CD	2.75	0.61
3:Q:67:ARG:NH1	3:Q:90:ASP:OD2	2.32	0.61
1:C:162:TYR:HB2	1:C:165:LEU:O	2.01	0.61
3:H:4:LEU:HD13	3:H:34:MET:HE1	1.81	0.61
1:A:182:ALA:HB2	2:B:562:ALA:HB2	1.81	0.61
1:C:189:ALA:O	1:C:190:LYS:HG3	2.00	0.61
1:A:63:LEU:HB3	2:B:585:LEU:HD11	1.82	0.61
3:H:6:GLN:H	3:H:114:GLN:NE2	1.98	0.61
2:B:575:ALA:O	1:E:164:ARG:NH2	2.34	0.60
4:N:29:ILE:HD11	4:N:71:PHE:CE2	2.36	0.60
4:L:2:ILE:HD12	4:L:27:GLN:HB2	1.82	0.60
3:Q:100:HIS:HB3	3:Q:108:HIS:HB3	1.83	0.60
1:C:97:VAL:HG13	1:C:166:ALA:HB3	1.83	0.60
4:R:32:TRP:HB3	4:R:91:TYR:HE1	1.66	0.60
2:F:572:PHE:HE2	2:F:587:ARG:NH1	2.00	0.60
1:E:57:LEU:HD12	1:E:62:GLN:HE21	1.67	0.59
3:H:35:SER:HB3	3:H:109:PHE:HZ	1.67	0.59
1:A:66:VAL:HA	1:A:101:ALA:HB3	1.83	0.59
2:F:527:ILE:N	2:F:527:ILE:HD12	2.16	0.59
4:L:33:LEU:HD23	4:L:34:ALA:N	2.17	0.59
2:B:529:LEU:O	2:B:529:LEU:HD12	2.03	0.59
3:Q:64:VAL:HB	3:Q:68:PHE:HD2	1.67	0.58
3:Q:168:LEU:HD21	3:Q:191:VAL:HG21	1.85	0.58
4:R:106:LYS:HD3	4:R:139:TYR:CD2	2.37	0.58
3:M:13:GLN:HB3	3:M:14:PRO:HD2	1.86	0.58
5:G:2:NAG:H3	5:G:2:NAG:C8	2.34	0.57
3:H:52:SER:O	3:H:72:ARG:NH1	2.37	0.57
4:N:52:SER:OG	6:J:8:NAG:N2	2.37	0.57
2:F:527:ILE:CG2	4:L:95:PRO:HD3	2.33	0.57
4:R:144:LYS:NZ	4:R:146:GLN:OE1	2.36	0.57
3:M:135:PRO:HG3	3:M:147:LEU:HB3	1.86	0.57
4:N:27:GLN:HG3	4:R:189:LYS:NZ	2.20	0.56
1:E:63:LEU:HB3	2:F:585:LEU:HD11	1.86	0.56
1:E:111:LEU:HD12	1:E:170:ILE:HG21	1.87	0.56
2:B:551:GLN:HG2	2:B:554:LEU:HD13	1.87	0.56
3:H:35:SER:HB3	3:H:109:PHE:CZ	2.40	0.56
1:A:64:ARG:HE	1:A:64:ARG:HA	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:32:TRP:HB3	4:R:91:TYR:CE1	2.40	0.56
8:C:300:NAG:H3	8:C:300:NAG:H83	1.88	0.56
1:E:160:PHE:O	1:E:162:TYR:HD2	1.89	0.55
4:N:29:ILE:HD11	4:N:71:PHE:HE2	1.69	0.55
3:H:164:ASN:HB3	3:H:167:ALA:HB3	1.89	0.55
3:H:83:MET:HB3	3:H:86:LEU:HD21	1.88	0.55
4:N:119:PRO:HD3	4:N:131:VAL:HG22	1.89	0.55
4:R:35:TRP:HB2	4:R:48:ILE:HG22	1.89	0.55
1:A:34:PRO:HD2	2:B:565:THR:HG23	1.87	0.55
3:H:91:THR:HG23	3:H:119:THR:HA	1.89	0.55
3:Q:114:GLN:OE1	3:Q:114:GLN:N	2.37	0.55
1:A:126:PRO:HD2	1:A:129:ILE:HD12	1.89	0.55
1:E:33:ILE:HB	2:F:588:LYS:NZ	2.22	0.55
4:N:154:GLN:HB3	4:N:157:ASN:HD21	1.71	0.55
1:A:97:VAL:O	1:A:166:ALA:N	2.33	0.55
4:L:102:LYS:NZ	4:L:141:ARG:HH22	2.04	0.55
3:M:29:PHE:CE1	3:M:72:ARG:CZ	2.87	0.55
1:E:162:TYR:CE1	1:E:171:TYR:HD2	2.24	0.55
1:C:95:LYS:NZ	2:D:574:ARG:HA	2.22	0.54
1:E:113:ILE:HG22	1:E:121:CYS:SG	2.47	0.54
1:C:126:PRO:HD2	1:C:129:ILE:HD12	1.88	0.54
3:M:114:GLN:OE1	3:M:114:GLN:N	2.37	0.54
4:N:12:SER:HB3	4:N:106:LYS:HB2	1.90	0.54
2:F:525:ALA:HB1	2:F:527:ILE:HD11	1.90	0.54
4:N:202:SER:HB3	4:R:11:LEU:HD13	1.90	0.54
3:M:101:ARG:NH1	6:J:3:BMA:H5	2.22	0.53
3:H:99:ASP:HA	3:H:108:HIS:O	2.08	0.53
1:A:162:TYR:HB2	1:A:165:LEU:O	2.09	0.53
2:B:597:TRP:CE2	2:D:597:TRP:HB3	2.44	0.53
1:C:72:GLY:HA3	2:D:559:ARG:NH2	2.23	0.53
1:A:111:LEU:HD12	1:A:170:ILE:HG21	1.91	0.52
3:H:147:LEU:HD13	3:H:220:VAL:HG11	1.90	0.52
1:E:112:GLU:O	1:E:142:SER:HA	2.10	0.52
3:H:157:GLU:HB3	3:H:158:PRO:HA	1.91	0.52
3:H:40:ALA:HB3	3:H:43:LYS:HB2	1.92	0.52
4:N:137:ASN:HA	4:N:171:THR:HB	1.91	0.52
3:H:6:GLN:N	3:H:114:GLN:HE22	2.06	0.52
3:M:99:ASP:HA	3:M:108:HIS:O	2.09	0.52
4:N:29:ILE:HD13	4:N:32:TRP:O	2.10	0.52
3:Q:22:CYS:HB3	3:Q:79:LEU:HB3	1.92	0.52
2:B:527:ILE:HG21	4:N:93:SER:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:160:PHE:HB2	1:E:162:TYR:HE2	1.75	0.51
3:M:164:ASN:HB2	3:M:167:ALA:HB3	1.91	0.51
2:B:531:TRP:NE1	2:D:567:GLN:HG2	2.25	0.51
4:L:102:LYS:HZ2	4:L:141:ARG:NH2	2.05	0.51
1:E:97:VAL:HG13	1:E:166:ALA:HB3	1.92	0.51
3:M:101:ARG:HH22	6:J:5:NAG:H61	1.76	0.51
1:C:43:LEU:HD21	2:D:557:GLY:HA3	1.92	0.51
3:H:100:HIS:HB2	3:H:110:ASP:HB3	1.92	0.51
3:M:73:ASP:OD2	3:M:76:LYS:HE2	2.10	0.51
4:R:108:THR:CG2	4:R:109:VAL:N	2.73	0.51
4:R:39:LYS:HG2	4:R:84:ALA:HB2	1.92	0.51
3:M:175:PHE:HA	4:N:163:THR:HG22	1.92	0.50
3:M:40:ALA:HB3	3:M:43:LYS:HB2	1.93	0.50
1:C:114:LYS:HE3	1:C:120:GLU:OE2	2.12	0.50
2:D:515:LEU:HB3	2:D:548:MET:HB2	1.94	0.50
3:M:14:PRO:HD3	3:M:122:SER:CB	2.42	0.50
1:A:64:ARG:NE	1:A:64:ARG:HA	2.27	0.50
3:Q:13:GLN:HB3	3:Q:14:PRO:HD2	1.93	0.50
3:Q:156:PRO:HD2	3:Q:211:PRO:HG2	1.93	0.50
1:C:74:GLY:HA3	2:D:510:LYS:HB2	1.94	0.50
1:E:57:LEU:HD12	1:E:62:GLN:NE2	2.27	0.50
3:Q:64:VAL:HB	3:Q:68:PHE:CD2	2.47	0.49
3:H:64:VAL:HB	3:H:68:PHE:CD2	2.47	0.49
2:F:537:PRO:HG2	2:F:542:ILE:HG22	1.94	0.49
4:N:33:LEU:HD23	4:N:90:GLN:HB3	1.94	0.49
4:N:47:LEU:HD11	4:N:62:PHE:HB3	1.95	0.49
4:N:48:ILE:HG13	4:N:54:LEU:HD23	1.94	0.49
3:M:29:PHE:CE1	3:M:72:ARG:NE	2.81	0.49
1:C:164:ARG:HB2	2:F:577:THR:HG21	1.95	0.49
3:M:61:ALA:HB3	3:M:64:VAL:HB	1.95	0.49
2:B:582:PHE:CE2	2:D:578:GLU:HG2	2.49	0.48
1:A:130:ARG:HH11	1:C:93:PRO:CB	2.24	0.48
2:D:560:GLN:HA	3:M:103:TRP:HH2	1.79	0.48
2:D:537:PRO:HG2	2:D:542:ILE:HG22	1.96	0.48
2:B:531:TRP:CD1	2:D:567:GLN:HG2	2.49	0.48
1:C:78:ASP:N	1:C:78:ASP:OD1	2.46	0.48
3:M:110:ASP:OD1	3:M:111:TYR:N	2.47	0.48
2:F:527:ILE:HD12	2:F:527:ILE:H	1.79	0.48
2:B:567:GLN:HG3	2:F:531:TRP:CD1	2.49	0.48
3:M:36:TRP:CE2	3:M:81:LEU:HB2	2.49	0.47
4:N:11:LEU:HD13	4:R:202:SER:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:7:SER:OG	4:R:8:PRO:HD3	2.14	0.47
3:H:128:PRO:HB3	3:H:154:TYR:HB3	1.95	0.47
1:A:130:ARG:HH11	1:C:93:PRO:HB3	1.78	0.47
2:D:531:TRP:HZ3	1:E:157:GLY:HA3	1.80	0.47
1:E:89:ARG:HB3	1:E:153:PHE:CD1	2.48	0.47
4:R:4:LEU:HA	4:R:25:ALA:HA	1.96	0.47
1:A:89:ARG:HB3	1:A:153:PHE:CD1	2.50	0.47
3:Q:99:ASP:HA	3:Q:108:HIS:O	2.15	0.47
3:Q:164:ASN:HB2	3:Q:167:ALA:HB3	1.95	0.47
3:M:72:ARG:HG3	3:M:79:LEU:HD12	1.93	0.47
1:A:73:ASN:HB3	2:B:559:ARG:HD3	1.97	0.47
3:M:175:PHE:HE1	3:M:190:VAL:HG22	1.78	0.47
1:C:63:LEU:O	1:C:64:ARG:NH1	2.48	0.47
3:M:91:THR:HG23	3:M:119:THR:HA	1.96	0.47
2:B:529:LEU:HD21	4:N:32:TRP:CE3	2.49	0.47
4:R:108:THR:O	4:R:139:TYR:CE2	2.68	0.47
1:E:55:ASP:OD1	2:F:596:ARG:NH2	2.48	0.47
3:H:51:ILE:HD13	3:H:72:ARG:HG3	1.97	0.47
2:D:538:ALA:O	2:D:542:ILE:HG23	2.14	0.46
1:C:133:PRO:HB3	2:D:543:TYR:CE2	2.51	0.46
3:Q:102:VAL:HG21	3:Q:106:GLY:CA	2.46	0.46
1:A:154:HIS:CE1	1:A:156:GLU:HB2	2.51	0.46
1:A:99:TYR:CZ	1:A:161:LEU:HD22	2.50	0.46
3:Q:45:LEU:HB2	4:R:97:PHE:CG	2.51	0.46
3:M:64:VAL:HG13	3:M:68:PHE:HB2	1.97	0.46
4:R:165:GLN:HG2	4:R:172:TYR:CZ	2.51	0.46
3:H:48:VAL:HG13	3:H:68:PHE:CE2	2.50	0.46
1:A:51:LEU:HD22	2:B:595:GLN:HG2	1.98	0.46
1:A:78:ASP:N	1:A:78:ASP:OD1	2.49	0.46
3:M:100:HIS:CD2	3:M:101:ARG:HG3	2.51	0.46
4:N:185:TYR:HA	4:N:191:TYR:OH	2.15	0.46
3:Q:122:SER:O	3:Q:122:SER:OG	2.34	0.46
1:C:189:ALA:O	1:C:190:LYS:CG	2.63	0.45
3:M:81:LEU:HD12	3:M:83:MET:HG2	1.98	0.45
3:Q:110:ASP:OD1	3:Q:111:TYR:N	2.49	0.45
3:Q:6:GLN:H	3:Q:114:GLN:NE2	2.14	0.45
1:C:38:ILE:O	1:C:187:PRO:HG3	2.16	0.45
1:A:155:LYS:NZ	6:I:8:NAG:O6	2.49	0.45
4:L:7:SER:OG	4:L:8:PRO:HD3	2.15	0.45
3:Q:36:TRP:CE2	3:Q:81:LEU:HB2	2.51	0.45
1:C:187:PRO:CB	1:C:190:LYS:HE3	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:525:ALA:HB1	2:F:527:ILE:HD13	1.95	0.45
1:C:57:LEU:HB3	2:F:594:LEU:HD22	1.98	0.45
3:H:15:GLY:HA2	3:H:85:SER:HA	1.99	0.45
4:L:137:ASN:HA	4:L:171:THR:HB	1.98	0.45
1:A:88:PHE:HA	1:A:152:ALA:HA	1.98	0.45
1:A:87:GLY:O	1:A:153:PHE:N	2.36	0.45
3:M:83:MET:HB3	3:M:86:LEU:HD21	1.97	0.45
4:N:35:TRP:HB2	4:N:48:ILE:HG22	1.98	0.45
2:D:593:LEU:HD21	2:F:594:LEU:HD23	1.99	0.45
3:H:153:ASP:HA	3:H:184:LEU:HB3	1.99	0.45
3:H:175:PHE:HA	4:L:163:THR:HG22	1.98	0.45
4:N:27:GLN:CG	4:R:189:LYS:NZ	2.80	0.45
2:D:597:TRP:CE2	2:F:597:TRP:HB3	2.52	0.44
3:H:110:ASP:OD1	3:H:111:TYR:N	2.50	0.44
3:M:193:VAL:HG11	3:M:203:TYR:CE2	2.52	0.44
3:Q:135:PRO:HG2	3:Q:222:PRO:HB3	1.99	0.44
2:B:534:TYR:O	1:C:89:ARG:NH2	2.47	0.44
3:M:132:PRO:CB	3:M:220:VAL:HG22	2.48	0.44
4:R:169:ASP:O	4:R:171:THR:HG23	2.17	0.44
4:L:102:LYS:HZ3	4:L:141:ARG:NH2	2.16	0.44
3:M:60:TYR:CZ	3:M:70:ILE:HG22	2.52	0.44
3:H:112:TRP:HE1	4:L:36:TYR:HE2	1.66	0.44
4:N:6:GLN:NE2	4:N:88:CYS:SG	2.90	0.44
4:R:33:LEU:HD13	4:R:34:ALA:N	2.32	0.44
1:C:37:VAL:HG12	1:C:185:ILE:HD12	2.00	0.44
4:L:154:GLN:HB3	4:L:157:ASN:HD21	1.82	0.44
4:L:165:GLN:HG2	4:L:172:TYR:CE1	2.52	0.44
1:A:52:VAL:HG12	1:A:54:ARG:H	1.83	0.44
3:H:61:ALA:HB3	3:H:64:VAL:HG22	1.98	0.44
4:L:90:GLN:N	4:L:90:GLN:OE1	2.51	0.44
1:A:122:LEU:HB2	1:A:172:ARG:HB2	1.99	0.44
4:R:36:TYR:CZ	4:R:46:LEU:HD23	2.53	0.44
3:Q:12:VAL:HG23	3:Q:120:VAL:HA	2.00	0.44
4:R:154:GLN:HB3	4:R:157:ASN:HD21	1.83	0.44
3:M:35:SER:HB3	3:M:109:PHE:CZ	2.53	0.43
3:Q:40:ALA:HB3	3:Q:43:LYS:HB2	1.99	0.43
3:Q:83:MET:HB3	3:Q:86:LEU:HD21	1.98	0.43
1:C:69:ASN:ND2	1:C:105:ALA:HB2	2.33	0.43
1:E:160:PHE:O	1:E:162:TYR:CE2	2.71	0.43
2:F:531:TRP:HH2	6:I:1:NAG:H83	1.84	0.43
1:C:51:LEU:HD22	2:D:595:GLN:HG3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:567:GLN:HG3	2:F:531:TRP:NE1	2.33	0.43
3:H:29:PHE:CE1	3:H:72:ARG:NH2	2.86	0.43
3:H:4:LEU:HD13	3:H:34:MET:CE	2.46	0.43
4:R:112:PRO:HB3	4:R:138:PHE:HB3	2.01	0.43
3:M:100:HIS:HB2	3:M:110:ASP:N	2.34	0.43
2:F:525:ALA:C	2:F:527:ILE:HD12	2.38	0.43
1:C:49:ASP:OD1	1:C:50:LYS:N	2.52	0.43
3:M:22:CYS:HB3	3:M:79:LEU:HB3	2.00	0.43
1:C:187:PRO:HB2	1:C:190:LYS:CE	2.47	0.43
4:R:4:LEU:HD22	4:R:23:CYS:SG	2.59	0.43
2:D:551:GLN:HG3	2:D:554:LEU:H	1.83	0.42
1:A:115:LYS:HB3	1:A:116:PRO:HD2	2.01	0.42
1:A:97:VAL:HG13	1:A:166:ALA:HB3	2.01	0.42
3:Q:5:VAL:HA	3:Q:114:GLN:HE22	1.84	0.42
1:A:111:LEU:HG	1:A:176:PHE:HE1	1.84	0.42
3:H:98:LYS:O	3:H:109:PHE:HA	2.19	0.42
3:M:100:HIS:HE1	4:N:55:GLU:OE1	2.03	0.42
3:Q:193:VAL:HG11	3:Q:203:TYR:CE1	2.54	0.42
3:Q:34:MET:HG3	3:Q:97:ALA:O	2.18	0.42
4:R:200:LEU:HD13	4:R:204:VAL:HG23	2.02	0.42
7:K:3:BMA:H62	7:K:6:MAN:H2	1.51	0.42
3:Q:61:ALA:HB3	3:Q:64:VAL:HG22	2.02	0.42
1:E:34:PRO:HD2	2:F:565:THR:HG23	2.01	0.42
4:R:112:PRO:HD2	4:R:200:LEU:HG	2.02	0.42
3:M:202:THR:HB	3:M:219:LYS:HE3	2.01	0.42
3:Q:67:ARG:NH1	3:Q:68:PHE:CZ	2.88	0.42
4:R:104:GLU:OE2	4:R:172:TYR:OH	2.37	0.42
1:C:132:PHE:HE2	1:C:161:LEU:HD13	1.84	0.42
2:B:521:GLN:HG2	2:B:524:GLY:HA3	2.01	0.42
1:E:151:PHE:HB2	1:E:153:PHE:CE1	2.54	0.42
4:N:31:SER:HB3	6:J:8:NAG:O7	2.20	0.42
4:L:139:TYR:O	4:L:197:HIS:HE1	2.03	0.41
3:M:14:PRO:HD3	3:M:122:SER:HB2	2.02	0.41
4:R:61:ARG:HD2	4:R:77:SER:O	2.19	0.41
1:E:115:LYS:HB3	1:E:116:PRO:HD2	2.01	0.41
3:M:61:ALA:O	3:M:65:LYS:N	2.53	0.41
4:L:90:GLN:HG2	4:L:90:GLN:O	2.21	0.41
3:Q:163:TRP:CZ3	3:Q:205:CYS:HB3	2.56	0.41
3:Q:202:THR:HB	3:Q:219:LYS:HE3	2.02	0.41
3:Q:36:TRP:CG	3:Q:81:LEU:HD22	2.56	0.41
4:R:48:ILE:HG13	4:R:54:LEU:HD23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:VAL:HB	2:B:580:ARG:HG2	2.02	0.41
4:N:39:LYS:HG2	4:N:84:ALA:HB2	2.01	0.41
1:C:115:LYS:HB3	1:C:116:PRO:HD2	2.03	0.41
1:C:154:HIS:CD2	1:C:156:GLU:HB2	2.55	0.41
4:L:123:GLN:HG2	4:L:128:THR:O	2.21	0.41
4:L:63:SER:O	4:L:73:LEU:HD12	2.20	0.41
4:N:47:LEU:HD21	4:N:62:PHE:CG	2.56	0.41
1:A:64:ARG:HG2	1:A:194:PHE:HE2	1.85	0.41
3:H:51:ILE:HB	3:H:70:ILE:HD13	2.02	0.41
3:M:51:ILE:HB	3:M:70:ILE:HD13	2.03	0.41
2:B:529:LEU:HD21	4:N:32:TRP:CD2	2.56	0.41
4:R:185:TYR:HA	4:R:191:TYR:OH	2.21	0.41
2:B:603:ILE:HB	2:F:612:PRO:HA	2.02	0.41
4:L:112:PRO:HB3	4:L:138:PHE:HB3	2.03	0.41
2:F:527:ILE:HB	4:L:93:SER:HA	2.03	0.41
4:N:200:LEU:HD13	4:N:204:VAL:HG23	2.03	0.41
3:Q:154:TYR:HB2	3:Q:209:HIS:CD2	2.56	0.41
3:M:10:THR:HB	3:M:18:LEU:HD21	2.03	0.40
2:B:576:THR:HG21	2:B:581:THR:HG21	2.03	0.40
4:N:106:LYS:HE3	4:N:140:PRO:HA	2.02	0.40
3:M:36:TRP:CZ2	3:M:81:LEU:HB2	2.56	0.40
2:B:570:GLN:HG3	2:F:531:TRP:HE3	1.86	0.40
2:F:521:GLN:HB2	2:F:544:ILE:HG21	2.03	0.40
3:M:72:ARG:CG	3:M:79:LEU:HD12	2.38	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	161/163 (99%)	157 (98%)	4 (2%)	0	<b>100</b> <b>100</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	157/163 (96%)	152 (97%)	5 (3%)	0	100	100
1	E	154/163 (94%)	150 (97%)	4 (3%)	0	100	100
2	B	104/111 (94%)	101 (97%)	3 (3%)	0	100	100
2	D	102/111 (92%)	99 (97%)	3 (3%)	0	100	100
2	F	101/111 (91%)	97 (96%)	4 (4%)	0	100	100
3	H	209/233 (90%)	205 (98%)	4 (2%)	0	100	100
3	M	213/233 (91%)	206 (97%)	7 (3%)	0	100	100
3	Q	220/233 (94%)	215 (98%)	5 (2%)	0	100	100
4	L	206/213 (97%)	200 (97%)	6 (3%)	0	100	100
4	N	207/213 (97%)	204 (99%)	3 (1%)	0	100	100
4	R	209/213 (98%)	204 (98%)	5 (2%)	0	100	100
All	All	2043/2160 (95%)	1990 (97%)	53 (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 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	134/134 (100%)	133 (99%)	1 (1%)	84	90
1	C	130/134 (97%)	130 (100%)	0	100	100
1	E	128/134 (96%)	128 (100%)	0	100	100
2	B	86/90 (96%)	86 (100%)	0	100	100
2	D	85/90 (94%)	85 (100%)	0	100	100
2	F	84/90 (93%)	84 (100%)	0	100	100
3	H	176/194 (91%)	175 (99%)	1 (1%)	86	92
3	M	180/194 (93%)	178 (99%)	2 (1%)	73	85
3	Q	183/194 (94%)	180 (98%)	3 (2%)	62	79
4	L	184/187 (98%)	183 (100%)	1 (0%)	88	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	N	185/187 (99%)	185 (100%)	0	100	100
4	R	185/187 (99%)	182 (98%)	3 (2%)	62	79
All	All	1740/1815 (96%)	1729 (99%)	11 (1%)	86	92

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
3	H	72	ARG
4	L	91	TYR
3	M	27	PHE
3	M	111	TYR
3	Q	27	PHE
3	Q	67	ARG
3	Q	72	ARG
4	R	4	LEU
4	R	91	TYR
4	R	106	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 ⓘ

26 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
5	NAG	G	1	1,5	14,14,15	0.29	0	17,19,21	0.74	0
5	NAG	G	2	5	14,14,15	0.27	0	17,19,21	0.62	0
5	FUC	G	3	5	10,10,11	0.24	0	14,14,16	0.64	0
6	NAG	I	1	2,6	14,14,15	0.35	0	17,19,21	0.45	0
6	NAG	I	2	6	14,14,15	0.30	0	17,19,21	0.49	0
6	BMA	I	3	6	11,11,12	0.43	0	15,15,17	0.88	1 (6%)
6	MAN	I	4	6	11,11,12	1.10	1 (9%)	15,15,17	1.19	2 (13%)
6	NAG	I	5	6	14,14,15	0.24	0	17,19,21	0.55	0
6	GAL	I	6	6	11,11,12	0.57	0	15,15,17	0.97	0
6	MAN	I	7	6	11,11,12	1.05	1 (9%)	15,15,17	1.76	2 (13%)
6	NAG	I	8	6	14,14,15	0.32	0	17,19,21	0.45	0
6	NAG	J	1	2,6	14,14,15	0.34	0	17,19,21	0.42	0
6	NAG	J	2	6	14,14,15	0.26	0	17,19,21	0.47	0
6	BMA	J	3	6	11,11,12	0.54	0	15,15,17	0.92	1 (6%)
6	MAN	J	4	6	11,11,12	0.91	1 (9%)	15,15,17	1.18	2 (13%)
6	NAG	J	5	6	14,14,15	0.28	0	17,19,21	0.50	0
6	GAL	J	6	6	11,11,12	0.51	0	15,15,17	1.00	1 (6%)
6	MAN	J	7	6	11,11,12	1.10	1 (9%)	15,15,17	1.07	0
6	NAG	J	8	6	14,14,15	0.35	0	17,19,21	0.46	0
7	NAG	K	1	2,7	14,14,15	0.40	0	17,19,21	0.45	0
7	NAG	K	2	7	14,14,15	0.29	0	17,19,21	0.51	0
7	BMA	K	3	7	11,11,12	0.73	0	15,15,17	0.90	1 (6%)
7	MAN	K	4	7	11,11,12	0.79	0	15,15,17	1.23	2 (13%)
7	NAG	K	5	7	14,14,15	0.33	0	17,19,21	0.70	0
7	MAN	K	6	7	11,11,12	0.94	1 (9%)	15,15,17	1.10	2 (13%)
7	NAG	K	7	7	14,14,15	0.34	0	17,19,21	0.52	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
5	NAG	G	1	1,5	-	5/6/23/26	0/1/1/1
5	NAG	G	2	5	-	3/6/23/26	0/1/1/1
5	FUC	G	3	5	-	-	0/1/1/1
6	NAG	I	1	2,6	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	I	2	6	-	3/6/23/26	0/1/1/1
6	BMA	I	3	6	-	2/2/19/22	0/1/1/1
6	MAN	I	4	6	-	0/2/19/22	0/1/1/1
6	NAG	I	5	6	-	0/6/23/26	0/1/1/1
6	GAL	I	6	6	-	1/2/19/22	0/1/1/1
6	MAN	I	7	6	-	2/2/19/22	0/1/1/1
6	NAG	I	8	6	-	1/6/23/26	0/1/1/1
6	NAG	J	1	2,6	-	0/6/23/26	0/1/1/1
6	NAG	J	2	6	-	1/6/23/26	0/1/1/1
6	BMA	J	3	6	-	2/2/19/22	0/1/1/1
6	MAN	J	4	6	-	0/2/19/22	0/1/1/1
6	NAG	J	5	6	-	1/6/23/26	0/1/1/1
6	GAL	J	6	6	-	1/2/19/22	0/1/1/1
6	MAN	J	7	6	-	1/2/19/22	0/1/1/1
6	NAG	J	8	6	-	3/6/23/26	0/1/1/1
7	NAG	K	1	2,7	-	0/6/23/26	0/1/1/1
7	NAG	K	2	7	-	1/6/23/26	0/1/1/1
7	BMA	K	3	7	-	2/2/19/22	0/1/1/1
7	MAN	K	4	7	-	1/2/19/22	0/1/1/1
7	NAG	K	5	7	-	3/6/23/26	0/1/1/1
7	MAN	K	6	7	-	0/2/19/22	0/1/1/1
7	NAG	K	7	7	-	1/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	I	4	MAN	C1-C2	2.70	1.58	1.52
7	K	6	MAN	C1-C2	2.58	1.58	1.52
6	J	4	MAN	C1-C2	2.52	1.58	1.52
6	I	7	MAN	O5-C5	2.47	1.48	1.43
6	J	7	MAN	C2-C3	2.43	1.56	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	I	7	MAN	C1-O5-C5	5.94	120.23	112.19
7	K	4	MAN	C1-O5-C5	3.13	116.43	112.19
6	J	4	MAN	O2-C2-C3	-2.80	104.53	110.14
6	I	4	MAN	O2-C2-C1	2.68	114.63	109.15
7	K	4	MAN	O2-C2-C3	-2.44	105.24	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	J	3	BMA	C1-O5-C5	2.33	115.35	112.19
7	K	6	MAN	C1-O5-C5	2.26	115.25	112.19
6	I	7	MAN	O2-C2-C3	-2.23	105.67	110.14
7	K	3	BMA	C1-O5-C5	2.21	115.19	112.19
6	J	4	MAN	C1-O5-C5	2.19	115.16	112.19
7	K	6	MAN	O2-C2-C3	-2.16	105.81	110.14
6	J	6	GAL	C1-O5-C5	2.10	115.03	112.19
6	I	4	MAN	C1-O5-C5	2.07	114.99	112.19
6	I	3	BMA	C1-O5-C5	2.06	114.98	112.19

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	G	1	NAG	C8-C7-N2-C2
5	G	1	NAG	O7-C7-N2-C2
5	G	2	NAG	C8-C7-N2-C2
5	G	2	NAG	O7-C7-N2-C2
6	I	3	BMA	C4-C5-C6-O6
6	I	7	MAN	C4-C5-C6-O6
7	K	3	BMA	C4-C5-C6-O6
6	J	3	BMA	C4-C5-C6-O6
6	I	2	NAG	O5-C5-C6-O6
7	K	5	NAG	O5-C5-C6-O6
6	I	3	BMA	O5-C5-C6-O6
6	I	7	MAN	O5-C5-C6-O6
6	J	3	BMA	O5-C5-C6-O6
6	J	8	NAG	C8-C7-N2-C2
6	J	8	NAG	O7-C7-N2-C2
7	K	3	BMA	O5-C5-C6-O6
5	G	2	NAG	C1-C2-N2-C7
5	G	1	NAG	C1-C2-N2-C7
7	K	5	NAG	C4-C5-C6-O6
6	I	2	NAG	C4-C5-C6-O6
6	J	2	NAG	O5-C5-C6-O6
6	J	8	NAG	O5-C5-C6-O6
6	J	7	MAN	O5-C5-C6-O6
5	G	1	NAG	C4-C5-C6-O6
7	K	4	MAN	O5-C5-C6-O6
7	K	2	NAG	O5-C5-C6-O6
7	K	5	NAG	C3-C2-N2-C7
5	G	1	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	J	6	GAL	O5-C5-C6-O6
7	K	7	NAG	C3-C2-N2-C7
6	J	5	NAG	C3-C2-N2-C7
6	I	8	NAG	C1-C2-N2-C7
6	I	2	NAG	C1-C2-N2-C7
6	I	6	GAL	O5-C5-C6-O6

There are no ring outliers.

8 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	J	8	NAG	2	0
7	K	3	BMA	1	0
6	J	5	NAG	1	0
6	I	1	NAG	1	0
6	J	3	BMA	1	0
6	I	8	NAG	1	0
5	G	2	NAG	3	0
7	K	6	MAN	1	0

## 5.6 Ligand geometry

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
8	NAG	E	300	1	14,14,15	0.24	0	17,19,21	0.49	0
8	NAG	C	300	1	14,14,15	0.38	0	17,19,21	1.23	1 (5%)

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
8	NAG	E	300	1	-	2/6/23/26	0/1/1/1
8	NAG	C	300	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	300	NAG	C2-N2-C7	4.29	129.01	122.90

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	300	NAG	C8-C7-N2-C2
8	C	300	NAG	O7-C7-N2-C2
8	E	300	NAG	O5-C5-C6-O6
8	C	300	NAG	O5-C5-C6-O6
8	E	300	NAG	C3-C2-N2-C7
8	C	300	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	300	NAG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.