



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 20, 2017 – 05:44 PM EDT

PDB ID : 1HZH  
Title : CRYSTAL STRUCTURE OF THE INTACT HUMAN IGG B12 WITH BROAD AND POTENT ACTIVITY AGAINST PRIMARY HIV-1 ISOLATES: A TEMPLATE FOR HIV VACCINE DESIGN  
Authors : Saphire, E.O.; Burton, D.R.; Wilson, I.A.  
Deposited on : 2001-01-24  
Resolution : 2.70 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

<http://wwpdb.org/validation/2016/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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20029077
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20029077

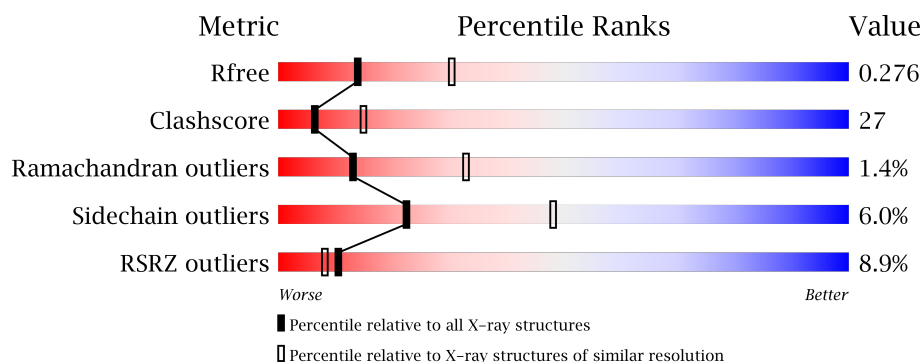
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
$R_{free}$	100719	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (2.70-2.70)

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	H	457	<div> <div>12%</div> <div>50%</div> <div>45%</div> <div>5%</div> </div>
1	K	457	<div> <div>8%</div> <div>62%</div> <div>32%</div> <div>• •</div> </div>
2	L	215	<div> <div>4%</div> <div>58%</div> <div>40%</div> <div>•</div> </div>
2	M	215	<div> <div>8%</div> <div>48%</div> <div>48%</div> <div>•</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	GAL	K	486	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 10647 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 IMMUNOGLOBULIN HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	457	Total	C	N	O	S	0	0	0
			3553	2252	600	685	16			
1	K	444	Total	C	N	O	S	0	0	0
			3466	2202	583	665	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	225	ALA	VAL	conflict	UNP P0DOX5
K	225	ALA	VAL	conflict	UNP P0DOX5

- Molecule 2 is a protein called IMMUNOGLOBULIN LIGHT CHAIN, Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	215	Total	C	N	O	S	0	0	0
			1668	1036	297	330	5			
2	M	215	Total	C	N	O	S	0	0	0
			1668	1036	297	330	5			

There are 2 discrepancies between the modelled and reference sequences:

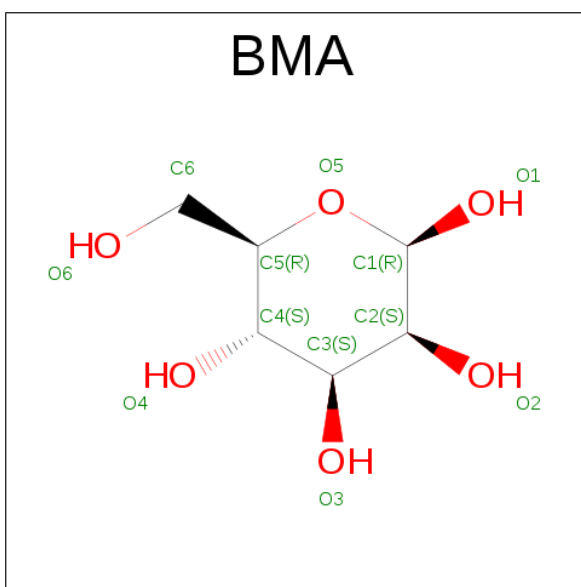
Chain	Residue	Modelled	Actual	Comment	Reference
L	202	ARG	SER	conflict	UNP Q8TCD0
M	202	ARG	SER	conflict	UNP Q8TCD0

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



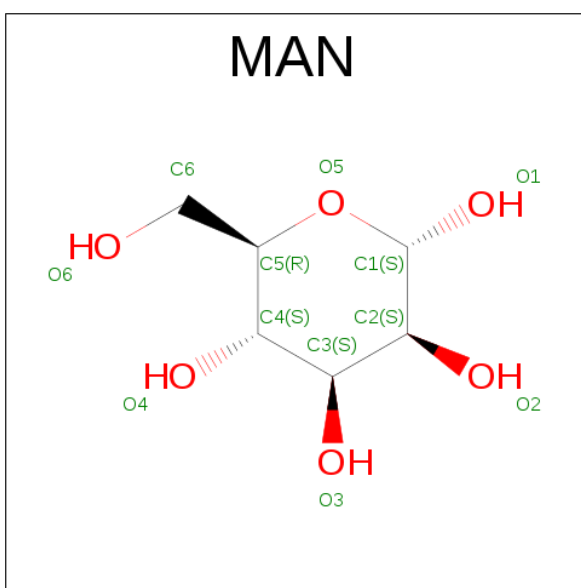
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	H	1	Total	C	N	O	0	0
			14	8	1	5		
3	H	1	Total	C	N	O	0	0
			14	8	1	5		
3	H	1	Total	C	N	O	0	0
			14	8	1	5		
3	H	1	Total	C	N	O	0	0
			14	8	1	5		
3	K	1	Total	C	N	O	0	0
			14	8	1	5		
3	K	1	Total	C	N	O	0	0
			14	8	1	5		
3	K	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is BETA-D-MANNOSE (three-letter code: BMA) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	H	1	Total	C	O	0	0
			11	6	5		
4	K	1	Total	C	O	0	0
			11	6	5		

- Molecule 5 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



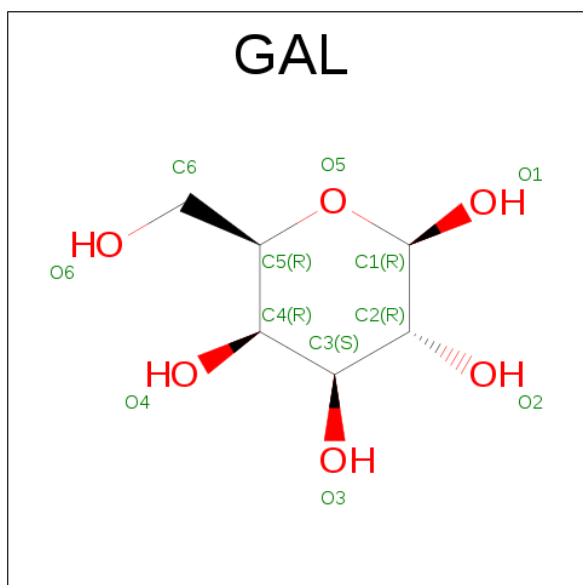
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	H	1	Total	C	O	0	0
			11	6	5		
5	H	1	Total	C	O	0	0
			11	6	5		

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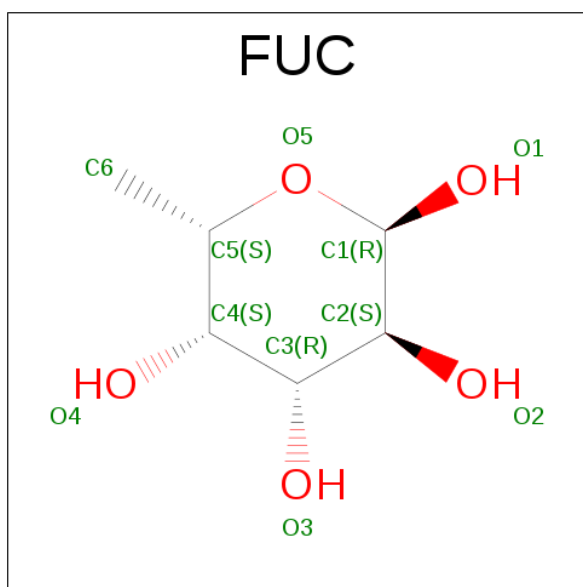
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	K	1	Total	C	O	0	0
			11	6	5		
5	K	1	Total	C	O	0	0
			11	6	5		

- Molecule 6 is BETA-D-GALACTOSE (three-letter code: GAL) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



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

- Molecule 7 is ALPHA-L-FUCOSE (three-letter code: FUC) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	K	1	Total	C	O	0	0
			10	6	4		

- Molecule 8 is water.

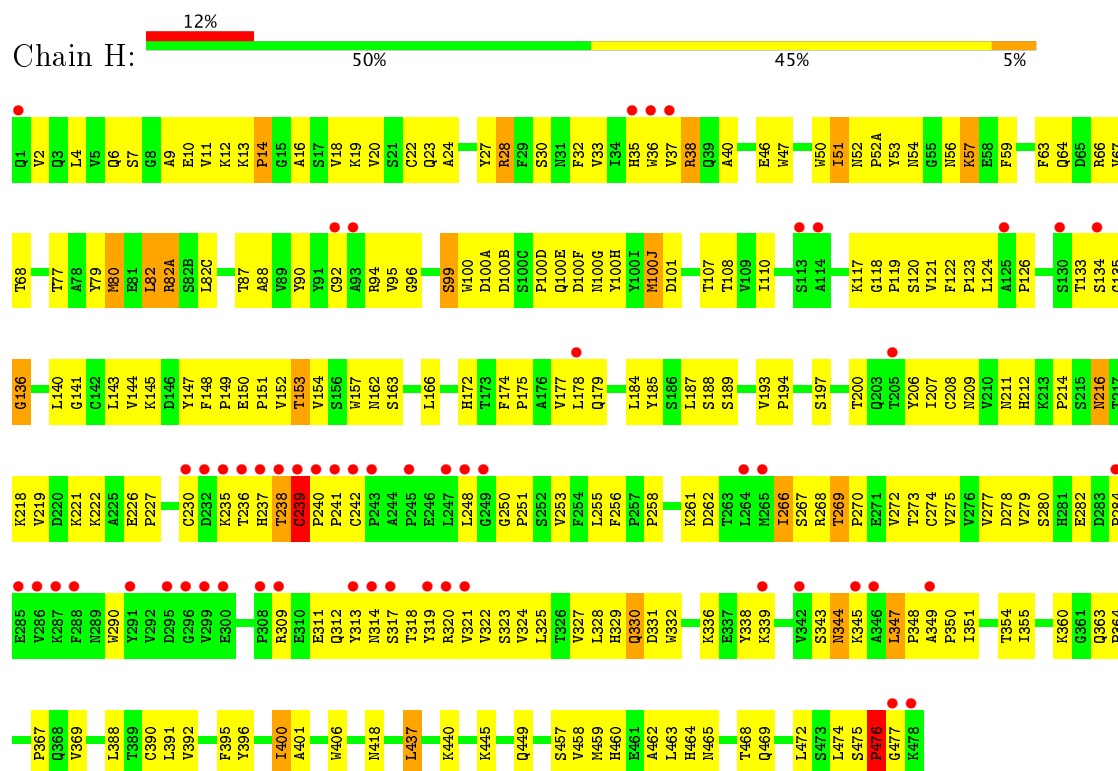
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	H	15	Total	O	0	0
			15	15		
8	K	38	Total	O	0	0
			38	38		
8	L	6	Total	O	0	0
			6	6		
8	M	12	Total	O	0	0
			12	12		



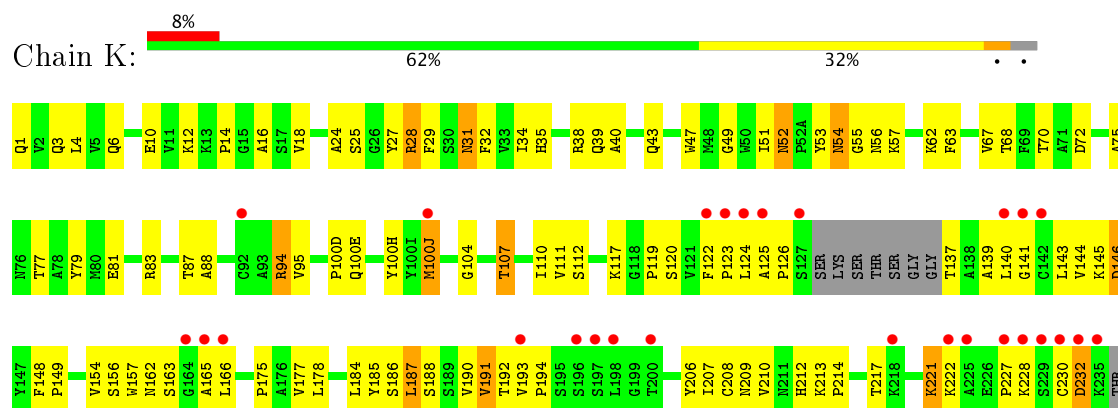
### 3 Residue-property plots

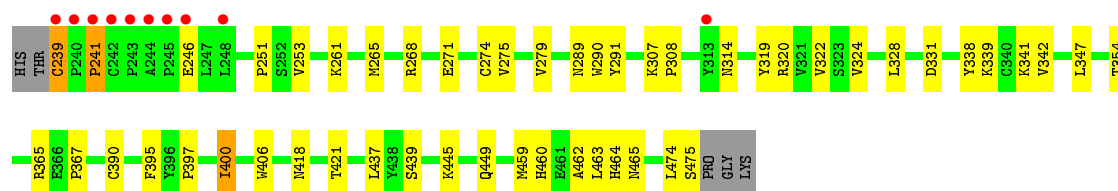
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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 ( $\text{RSRZ} > 2$ ). 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: IMMUNOGLOBULIN HEAVY CHAIN

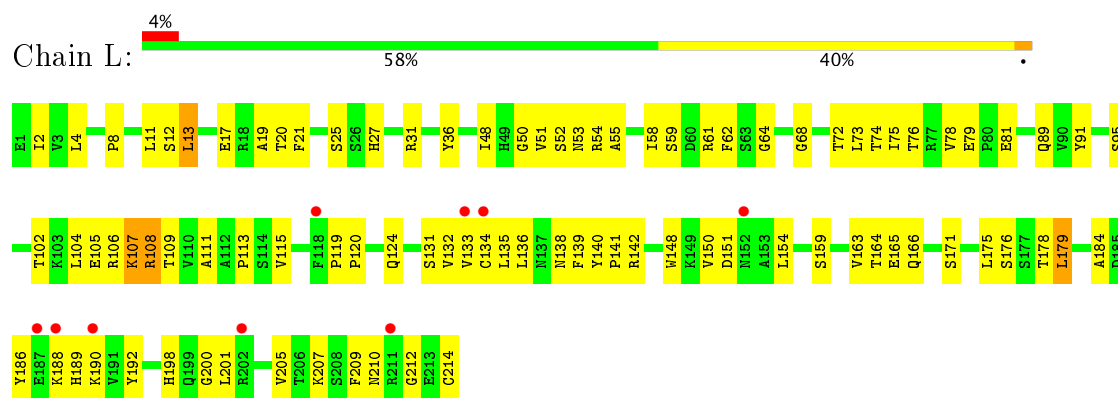


- Molecule 1: IMMUNOGLOBULIN HEAVY CHAIN





- Molecule 2: IMMUNOGLOBULIN LIGHT CHAIN, Uncharacterized protein



- Molecule 2: IMMUNOGLOBULIN LIGHT CHAIN, Uncharacterized protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	271.32Å 271.32Å 175.18Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.65 – 2.70 29.65 – 2.60	Depositor EDS
% Data completeness (in resolution range)	91.7 (29.65-2.70) 90.8 (29.65-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.84 (at 2.61Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, $R_{free}$	0.229 , 0.273 0.233 , 0.276	Depositor DCC
$R_{free}$ test set	6302 reflections (10.19%)	DCC
Wilson B-factor (Å <sup>2</sup> )	58.0	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 68.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.008 for $-1/3^*h+1/3^*k+4/3^*l, -k, 2/3^*h+1/3^*k+1/3^*l$ 0.012 for $-2/3^*h-1/3^*k-4/3^*l, -1/3^*h-2/3^*k+4/3^*l, -1/3^*h+1/3^*k+1/3^*l$ 0.006 for $-h, 1/3^*h-1/3^*k-4/3^*l, -1/3^*h-2/3^*k+1/3^*l$	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10647	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% 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: MAN, GAL, BMA, NAG, FUC

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	H	0.37	0/3654	0.62	0/4983
1	K	0.40	0/3563	0.64	0/4859
2	L	0.34	0/1704	0.60	0/2306
2	M	0.38	0/1704	0.63	0/2306
All	All	0.38	0/10625	0.62	0/14454

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	136	GLY	Mainchain

### 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	H	3553	0	3460	231	1
1	K	3466	0	3373	152	0
2	L	1668	0	1621	69	0
2	M	1668	0	1621	110	0
3	H	56	0	48	11	0
3	K	56	0	48	7	0
4	H	11	0	8	0	0
4	K	11	0	8	0	0
5	H	22	0	18	0	0
5	K	22	0	18	0	0
6	H	22	0	20	3	0
6	K	11	0	10	0	0
7	K	10	0	10	0	0
8	H	15	0	0	2	0
8	K	38	0	0	0	0
8	L	6	0	0	0	0
8	M	12	0	0	1	0
All	All	10647	0	10263	556	1

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 27.

All (556) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:261:LYS:HE2	1:K:265:MET:HE1	1.09	1.06
1:H:400:ILE:HD11	1:H:458:VAL:HG13	1.38	1.05
1:K:221:LYS:HE3	1:K:221:LYS:HA	1.39	1.04
2:M:1:GLU:HG3	2:M:2:ILE:H	1.18	1.03
2:M:100:GLN:NE2	2:M:100:GLN:H	1.56	1.03
1:H:277:VAL:HG11	3:H:480:NAG:O7	1.59	1.02
1:H:145:LYS:HE3	1:H:179:GLN:HE22	1.23	1.00
1:K:314:ASN:HD21	3:K:479:NAG:C1	1.75	0.98
1:H:27:TYR:HB2	1:H:28:ARG:HH21	1.30	0.95
1:K:28:ARG:HE	1:K:28:ARG:H	1.11	0.95
2:M:149:LYS:HB2	2:M:193:ALA:HB3	1.44	0.95
1:H:124:LEU:HD11	1:H:143:LEU:HB2	1.47	0.94
2:M:100:GLN:H	2:M:100:GLN:HE21	0.95	0.94
1:H:367:PRO:HB3	1:H:395:PHE:HB3	1.49	0.94
1:H:150:GLU:HB2	1:H:151:PRO:HA	1.50	0.94
2:L:11:LEU:HG	2:L:13:LEU:HD11	1.48	0.94
1:H:347:LEU:HD23	1:H:348:PRO:HD2	1.49	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:100:GLN:N	2:M:100:GLN:HE21	1.69	0.91
2:M:190:LYS:O	2:M:211:ARG:HB3	1.73	0.89
1:H:28:ARG:H	1:H:28:ARG:HE	0.89	0.88
1:H:28:ARG:NE	1:H:28:ARG:H	1.71	0.88
1:K:28:ARG:NE	1:K:28:ARG:H	1.72	0.88
1:H:121:VAL:HG21	1:H:219:VAL:HG11	1.52	0.88
2:M:16:GLY:HA2	2:M:77:ARG:HG3	1.57	0.87
1:K:261:LYS:CE	1:K:265:MET:HE1	2.01	0.85
1:K:212:HIS:HD2	1:K:214:PRO:HD2	1.42	0.85
2:M:39:LYS:HD3	2:M:84:ALA:HB2	1.56	0.85
1:H:28:ARG:N	1:H:28:ARG:HE	1.73	0.85
1:H:35:HIS:HD2	1:H:47:TRP:HE1	1.22	0.84
1:H:187:LEU:HD13	1:H:188:SER:N	1.93	0.84
2:M:188:LYS:N	2:M:211:ARG:HH12	1.74	0.84
1:H:339:LYS:HG2	1:H:354:THR:HG22	1.58	0.84
1:K:3:GLN:HB2	1:K:25:SER:HB2	1.58	0.83
2:L:55:ALA:O	2:L:58:ILE:HD13	1.80	0.81
1:H:314:ASN:HD21	3:H:479:NAG:C1	1.94	0.81
1:K:314:ASN:ND2	3:K:479:NAG:C1	2.45	0.79
1:K:275:VAL:HG22	1:K:322:VAL:HG22	1.64	0.79
1:K:54:ASN:ND2	1:K:56:ASN:H	1.80	0.78
1:K:94:ARG:HD3	1:K:95:VAL:O	1.83	0.78
1:H:460:HIS:CD2	1:H:462:ALA:H	2.00	0.78
1:H:66:ARG:HH21	1:H:82:LEU:HD11	1.49	0.77
1:K:63:PHE:HB3	1:K:67:VAL:HG21	1.64	0.77
3:H:483:NAG:H61	6:H:484:GAL:C1	2.15	0.77
1:H:400:ILE:HD13	1:H:401:ALA:N	1.98	0.77
2:M:1:GLU:HG3	2:M:2:ILE:N	1.98	0.77
1:K:126:PRO:HG3	1:K:140:LEU:HB3	1.67	0.77
2:M:105:GLU:HG3	2:M:173:TYR:OH	1.85	0.76
1:H:163:SER:H	1:H:209:ASN:HD21	1.30	0.76
1:H:212:HIS:HD2	1:H:214:PRO:HD2	1.50	0.75
1:H:51:ILE:HD13	1:H:52:ASN:N	2.02	0.75
1:K:320:ARG:NE	3:K:480:NAG:H81	2.02	0.75
2:L:19:ALA:HB3	2:L:75:ILE:HG12	1.69	0.75
1:K:400:ILE:HD12	1:K:460:HIS:HB2	1.68	0.74
1:H:256:PHE:CE2	3:H:486:NAG:H5	2.22	0.73
1:K:228:LYS:HE2	2:M:213:GLU:OE2	1.88	0.73
2:L:108:ARG:HD3	2:L:109:THR:O	1.89	0.73
1:K:289:ASN:HB2	1:K:341:LYS:HB3	1.70	0.73
1:K:87:THR:HG23	1:K:110:ILE:HA	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:17:GLU:O	2:L:78:VAL:HG23	1.89	0.72
2:M:151:ASP:HB2	2:M:189:HIS:HB3	1.70	0.72
1:K:145:LYS:HG2	1:K:146:ASP:OD1	1.90	0.71
1:H:30:SER:HA	1:H:52(A):PRO:HB2	1.70	0.71
2:M:202:ARG:O	2:M:202:ARG:HD3	1.91	0.71
1:H:35:HIS:CD2	1:H:47:TRP:HE1	2.07	0.71
1:H:145:LYS:HE3	1:H:179:GLN:NE2	2.01	0.71
1:H:256:PHE:CD2	3:H:486:NAG:H5	2.26	0.70
1:H:38:ARG:HD2	1:H:46:GLU:OE1	1.92	0.70
1:K:63:PHE:HB3	1:K:67:VAL:CG2	2.22	0.70
1:H:117:LYS:HG2	1:H:118:GLY:H	1.56	0.70
2:L:175:LEU:HD23	2:L:176:SER:N	2.07	0.69
2:M:181:LEU:HD12	2:M:185:ASP:HB2	1.74	0.69
1:H:193:VAL:HG22	1:H:194:PRO:HD2	1.74	0.69
1:H:162:ASN:ND2	1:H:207:ILE:H	1.91	0.69
2:M:187:GLU:HA	2:M:211:ARG:CZ	2.22	0.69
2:M:6:GLN:H	2:M:100:GLN:HE22	1.40	0.69
2:L:186:TYR:HA	2:L:192:TYR:OH	1.92	0.69
2:L:124:GLN:HE22	2:L:131:SER:HB2	1.58	0.69
1:K:193:VAL:HG13	1:K:194:PRO:HD2	1.75	0.68
1:H:33:VAL:HB	1:H:95:VAL:HG21	1.75	0.68
1:H:6:GLN:HE21	1:H:107:THR:HG23	1.57	0.68
1:K:139:ALA:HB2	1:K:192:THR:HG22	1.74	0.67
1:K:63:PHE:O	1:K:67:VAL:HG23	1.93	0.67
1:K:367:PRO:HB3	1:K:395:PHE:HB3	1.75	0.67
1:H:119:PRO:HD3	1:H:212:HIS:ND1	2.10	0.67
1:H:82:LEU:HD13	1:H:82(A):ARG:N	2.10	0.67
1:H:193:VAL:CG2	1:H:194:PRO:HD2	2.24	0.67
2:L:12:SER:HB3	2:L:105:GLU:CG	2.24	0.67
1:H:23:GLN:HG2	1:H:77:THR:OG1	1.95	0.66
1:H:63:PHE:HB3	1:H:67:VAL:CG2	2.25	0.66
1:K:261:LYS:HE2	1:K:265:MET:CE	2.05	0.66
1:H:163:SER:N	1:H:209:ASN:HD21	1.93	0.66
1:H:212:HIS:CD2	1:H:214:PRO:HD2	2.30	0.66
2:M:28(A):ILE:HD13	2:M:71:PHE:HE2	1.60	0.66
1:H:66:ARG:HA	1:H:82(A):ARG:NH1	2.11	0.66
1:H:33:VAL:HB	1:H:95:VAL:CG2	2.25	0.66
1:H:117:LYS:HG2	1:H:118:GLY:N	2.11	0.66
2:M:135:LEU:HD12	2:M:136:LEU:N	2.11	0.66
1:H:63:PHE:HB3	1:H:67:VAL:HG23	1.78	0.65
2:M:143:GLU:CD	2:M:143:GLU:H	2.00	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:95:VAL:HG12	1:H:96:GLY:N	2.11	0.65
2:M:189:HIS:O	2:M:211:ARG:HD3	1.96	0.65
1:H:122:PHE:CD1	2:L:124:GLN:HB2	2.32	0.65
1:H:100(B):ASP:HB2	1:H:100(F):ASP:HB2	1.79	0.64
1:K:117:LYS:HE3	1:K:146:ASP:O	1.97	0.64
1:H:2:VAL:HG12	1:H:27:TYR:HB3	1.78	0.64
2:M:125:LEU:O	2:M:183:LYS:HD2	1.98	0.64
1:H:330:GLN:CD	1:H:330:GLN:H	2.01	0.64
1:K:261:LYS:HD3	1:K:268:ARG:NH2	2.12	0.64
2:L:132:VAL:HB	2:L:179:LEU:HB3	1.80	0.64
2:M:188:LYS:H	2:M:211:ARG:HH12	1.43	0.64
1:K:35:HIS:HD2	1:K:47:TRP:HE1	1.43	0.64
1:K:54:ASN:HD21	1:K:56:ASN:HB2	1.63	0.64
1:K:178:LEU:HD13	1:K:185:TYR:CE2	2.33	0.64
2:M:155:GLN:NE2	2:M:158:ASN:HD21	1.96	0.64
1:K:137:THR:HG23	1:K:193:VAL:O	1.98	0.63
1:H:309:ARG:HG2	1:H:321:VAL:HG22	1.80	0.63
1:H:110:ILE:H	1:H:110:ILE:HD12	1.64	0.63
1:K:119:PRO:HD2	1:K:217:THR:HG21	1.79	0.63
2:M:200:GLY:O	2:M:201:LEU:HD12	1.98	0.63
1:H:145:LYS:CE	1:H:179:GLN:HE22	2.06	0.63
2:M:175:LEU:HD23	2:M:176:SER:N	2.14	0.63
1:K:212:HIS:CD2	1:K:214:PRO:HD2	2.31	0.62
2:M:113:PRO:HB3	2:M:139:PHE:HB3	1.81	0.62
1:K:162:ASN:HB2	1:K:165:ALA:HB3	1.81	0.62
1:H:6:GLN:NE2	1:H:107:THR:HG23	2.14	0.62
2:M:108:ARG:HD3	2:M:109:THR:O	1.99	0.62
2:M:151:ASP:CB	2:M:189:HIS:HB3	2.29	0.62
1:H:255:LEU:HD12	1:H:273:THR:O	2.00	0.61
1:H:278:ASP:OD1	3:H:479:NAG:H3	2.00	0.61
1:H:87:THR:HG23	1:H:110:ILE:HA	1.82	0.61
1:K:6:GLN:HE21	1:K:104:GLY:HA3	1.65	0.61
1:K:328:LEU:HD12	1:K:331:ASP:OD2	2.01	0.61
1:K:274:CYS:HB2	1:K:290:TRP:CH2	2.36	0.61
2:L:4:LEU:HD23	2:L:25:SER:HB3	1.83	0.61
1:H:258:PRO:HD3	1:H:272:VAL:HG22	1.83	0.61
1:H:390:CYS:HB2	1:H:406:TRP:CZ2	2.35	0.61
1:H:256:PHE:HE1	1:H:275:VAL:HG12	1.65	0.61
3:H:483:NAG:C6	6:H:484:GAL:C1	2.78	0.61
1:H:328:LEU:HB2	1:H:331:ASP:OD2	2.01	0.61
1:H:314:ASN:ND2	3:H:479:NAG:C1	2.64	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:279:VAL:HB	1:H:319:TYR:HB2	1.83	0.60
2:L:12:SER:HB3	2:L:105:GLU:HG2	1.83	0.60
2:L:36:TYR:CE1	2:L:89:GLN:HG2	2.36	0.60
1:H:238:THR:O	1:H:239:CYS:HB2	2.00	0.60
1:H:54:ASN:CG	1:H:56:ASN:HD22	2.05	0.60
1:H:82:LEU:HD12	1:H:82(C):LEU:HD23	1.82	0.60
2:L:201:LEU:HD13	2:L:205:VAL:HG23	1.82	0.60
1:K:122:PHE:HB3	2:M:121:SER:OG	2.02	0.60
1:K:460:HIS:CD2	1:K:462:ALA:H	2.19	0.60
1:K:100(D):PRO:O	1:K:100(E):GLN:HB2	2.01	0.60
1:K:47:TRP:CZ2	1:K:49:GLY:HA2	2.36	0.60
1:K:52:ASN:C	1:K:52:ASN:HD22	2.04	0.60
1:H:40:ALA:HA	1:H:88:ALA:HB2	1.84	0.60
1:K:339:LYS:HB2	1:K:354:THR:HG22	1.84	0.59
2:L:55:ALA:C	2:L:58:ILE:HD13	2.23	0.59
1:K:83:ARG:O	1:K:111:VAL:HG11	2.03	0.59
1:H:360:LYS:HE2	1:H:360:LYS:HA	1.84	0.59
2:M:124:GLN:HE22	2:M:131:SER:N	2.01	0.59
2:M:150:VAL:HG23	2:M:155:GLN:HB2	1.83	0.59
1:K:175:PRO:HG2	2:M:162:SER:OG	2.03	0.59
2:M:105:GLU:HG2	2:M:106:ARG:N	2.17	0.59
2:M:48:ILE:HD13	2:M:54:ARG:HA	1.83	0.59
1:K:1:GLN:HG3	1:K:1:GLN:O	2.02	0.59
2:M:145:LYS:HB2	2:M:197:THR:HB	1.85	0.58
1:H:126:PRO:HD3	1:H:140:LEU:HB3	1.84	0.58
1:H:187:LEU:HD13	1:H:188:SER:H	1.65	0.58
2:M:24:ARG:HD2	2:M:70:ASP:OD1	2.02	0.58
1:H:331:ASP:O	1:H:336:LYS:HB2	2.04	0.58
1:H:207:ILE:HG13	1:H:207:ILE:O	2.02	0.58
2:M:113:PRO:HD3	2:M:198:HIS:CD2	2.39	0.58
1:H:153:THR:OG1	1:H:211:ASN:HB3	2.04	0.57
2:M:16:GLY:HA2	2:M:77:ARG:CG	2.33	0.57
1:H:144:VAL:HB	1:H:187:LEU:HB3	1.84	0.57
1:H:207:ILE:HG22	1:H:222:LYS:HA	1.86	0.57
1:H:400:ILE:HD11	1:H:458:VAL:CG1	2.25	0.57
2:M:155:GLN:CD	2:M:179:LEU:HD11	2.25	0.57
1:H:59:PHE:CD2	1:H:64:GLN:HA	2.40	0.57
2:L:72:THR:HG22	2:L:73:LEU:N	2.19	0.57
1:K:54:ASN:HD22	1:K:56:ASN:H	1.52	0.57
2:M:192:TYR:HB2	2:M:209:PHE:CE1	2.40	0.57
1:H:162:ASN:HD21	1:H:206:TYR:HA	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:155:GLN:OE1	2:M:179:LEU:HD11	2.04	0.57
2:M:202:ARG:C	2:M:202:ARG:HD3	2.26	0.56
1:K:28:ARG:HG2	1:K:31:ASN:HB2	1.88	0.56
1:K:54:ASN:C	1:K:54:ASN:HD22	2.08	0.56
1:H:4:LEU:HD23	1:H:92:CYS:O	2.06	0.56
1:K:119:PRO:HB2	1:K:144:VAL:HG13	1.88	0.56
1:H:347:LEU:HD22	1:H:349:ALA:O	2.05	0.56
2:M:100:GLN:N	2:M:100:GLN:NE2	2.38	0.56
2:M:189:HIS:O	2:M:211:ARG:NH1	2.39	0.56
1:K:166:LEU:HD21	1:K:191:VAL:HG21	1.88	0.56
1:K:28:ARG:HE	1:K:28:ARG:N	1.92	0.56
1:H:162:ASN:HD21	1:H:207:ILE:H	1.52	0.56
1:H:270:PRO:HD3	1:H:329:HIS:CE1	2.41	0.56
1:H:329:HIS:HB2	1:H:330:GLN:OE1	2.05	0.56
1:H:339:LYS:HE2	1:H:354:THR:HG21	1.88	0.56
1:H:121:VAL:CG2	1:H:219:VAL:HG11	2.31	0.55
1:H:32:PHE:CG	1:H:94:ARG:HD2	2.41	0.55
1:H:400:ILE:HD13	1:H:401:ALA:H	1.71	0.55
1:H:347:LEU:HD23	1:H:348:PRO:CD	2.31	0.55
1:K:207:ILE:HG12	1:K:222:LYS:HA	1.88	0.55
2:M:115:VAL:O	2:M:116:PHE:HD2	1.89	0.55
1:K:6:GLN:HB2	1:K:107:THR:CG2	2.37	0.55
2:M:124:GLN:NE2	2:M:131:SER:N	2.55	0.55
2:M:155:GLN:HG2	2:M:156:SER:N	2.22	0.55
1:K:140:LEU:HD21	1:K:206:TYR:HD1	1.72	0.55
1:K:27:TYR:CB	1:K:28:ARG:HH21	2.19	0.55
1:K:221:LYS:HA	1:K:221:LYS:CE	2.24	0.54
2:M:131:SER:HA	2:M:179:LEU:O	2.07	0.54
1:H:178:LEU:HD13	1:H:185:TYR:CE1	2.43	0.54
1:H:82:LEU:HD12	1:H:82(C):LEU:CD2	2.36	0.54
1:K:239:CYS:O	1:K:239:CYS:SG	2.65	0.54
1:H:177:VAL:O	1:H:177:VAL:HG12	2.08	0.54
1:K:163:SER:HA	1:K:209:ASN:OD1	2.08	0.54
1:K:187:LEU:HD12	1:K:188:SER:N	2.22	0.54
1:K:141:GLY:HA2	1:K:157:TRP:CH2	2.42	0.54
2:L:108:ARG:NH1	2:L:111:ALA:HB2	2.22	0.54
2:L:4:LEU:CD2	2:L:25:SER:HB3	2.37	0.54
2:L:52:SER:HB3	2:L:64:GLY:O	2.06	0.54
2:M:175:LEU:C	2:M:175:LEU:HD23	2.27	0.54
1:H:95:VAL:HG13	1:H:100(G):ASN:O	2.07	0.54
1:K:52:ASN:ND2	1:K:53:TYR:H	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:110:ILE:N	1:H:110:ILE:HD12	2.23	0.54
1:H:19:LYS:HE2	1:H:79:TYR:CD2	2.43	0.54
1:H:251:PRO:HG2	1:H:347:LEU:HD12	1.90	0.54
2:L:19:ALA:O	2:L:74:THR:HA	2.08	0.54
2:L:59:SER:C	2:L:61:ARG:H	2.11	0.54
1:H:140:LEU:HD21	1:H:206:TYR:CD2	2.44	0.53
1:K:193:VAL:CG1	1:K:194:PRO:HD2	2.38	0.53
1:K:27:TYR:HB2	1:K:28:ARG:HH21	1.73	0.53
1:H:437:LEU:C	1:H:437:LEU:HD12	2.29	0.53
1:K:190:VAL:HG21	2:M:135:LEU:HD22	1.90	0.53
2:M:130:ALA:HB3	2:M:181:LEU:O	2.09	0.53
1:H:12:LYS:HB3	1:H:16:ALA:HB3	1.89	0.53
1:H:314:ASN:HD21	3:H:479:NAG:C2	2.22	0.53
1:H:37:VAL:HG13	1:H:46:GLU:O	2.09	0.53
1:H:4:LEU:HD12	1:H:24:ALA:HB2	1.91	0.53
1:H:7:SER:OG	1:H:20:VAL:HG13	2.09	0.53
1:K:52:ASN:HB3	1:K:54:ASN:HD21	1.73	0.53
1:H:99:SER:HB2	1:H:100(B):ASP:OD2	2.08	0.52
1:H:35:HIS:HD2	1:H:47:TRP:NE1	1.99	0.52
1:H:38:ARG:HG3	1:H:46:GLU:HB2	1.90	0.52
1:K:110:ILE:HD12	1:K:110:ILE:N	2.24	0.52
1:H:280:SER:HB2	1:H:282:GLU:OE1	2.08	0.52
1:H:255:LEU:HD23	1:H:355:ILE:HB	1.90	0.52
1:H:67:VAL:HG12	1:H:68:THR:N	2.24	0.52
2:M:141:PRO:HB2	2:M:143:GLU:OE2	2.08	0.52
2:L:31:ARG:NH2	2:L:51:VAL:HG11	2.24	0.52
2:M:6:GLN:H	2:M:100:GLN:NE2	2.06	0.52
1:H:290:TRP:HZ2	1:H:323:SER:HG	1.55	0.52
2:M:123:GLU:HA	2:M:126:LYS:HE2	1.92	0.52
2:M:191:VAL:HG12	2:M:192:TYR:N	2.25	0.52
2:M:202:ARG:O	2:M:204:PRO:HD3	2.09	0.52
1:K:10:GLU:HG3	1:K:18:VAL:CG2	2.40	0.52
2:L:140:TYR:CE1	2:L:141:PRO:HG3	2.45	0.52
2:L:62:PHE:CE2	2:L:75:ILE:HD12	2.44	0.52
1:H:174:PHE:O	1:H:187:LEU:HD22	2.09	0.52
1:H:66:ARG:HA	1:H:82(A):ARG:HH12	1.74	0.52
1:H:226:GLU:HG3	1:H:227:PRO:HD2	1.91	0.52
1:H:27:TYR:CB	1:H:28:ARG:HH21	2.12	0.52
1:H:95:VAL:CG1	1:H:96:GLY:N	2.73	0.52
2:L:79:GLU:HB3	2:L:81:GLU:OE1	2.10	0.52
1:H:400:ILE:HD13	1:H:401:ALA:C	2.30	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:188:LYS:H	2:M:211:ARG:NH1	2.06	0.51
3:H:483:NAG:H5	6:H:484:GAL:O2	2.10	0.51
1:K:400:ILE:CD1	1:K:460:HIS:HB2	2.38	0.51
2:L:201:LEU:HD13	2:L:205:VAL:CG2	2.40	0.51
2:L:184:ALA:O	2:L:188:LYS:HG3	2.09	0.51
1:H:100:TRP:CZ3	1:H:100(A):ASP:HB3	2.45	0.51
1:K:279:VAL:HB	1:K:319:TYR:HB2	1.93	0.51
1:H:141:GLY:HA2	1:H:157:TRP:CH2	2.46	0.51
1:H:13:LYS:HB3	1:H:14:PRO:HD2	1.92	0.51
1:H:339:LYS:CG	1:H:354:THR:HG22	2.34	0.51
1:H:35:HIS:CD2	1:H:50:TRP:HB3	2.46	0.51
1:H:330:GLN:OE1	1:H:330:GLN:N	2.40	0.51
2:L:107:LYS:HD3	2:L:140:TYR:OH	2.11	0.51
1:K:140:LEU:HD21	1:K:206:TYR:CD1	2.46	0.51
1:K:191:VAL:O	1:K:191:VAL:HG13	2.11	0.51
1:K:24:ALA:HB1	1:K:27:TYR:CE1	2.46	0.51
1:K:68:THR:HB	1:K:81:GLU:HB3	1.92	0.51
1:K:154:VAL:HG12	1:K:210:VAL:HG22	1.92	0.51
2:L:190:LYS:O	2:L:210:ASN:HA	2.11	0.51
1:H:11:VAL:HG22	1:H:110:ILE:HD13	1.92	0.50
1:K:209:ASN:ND2	1:K:209:ASN:N	2.59	0.50
1:K:100(E):GLN:HG2	1:K:100(H):TYR:CD2	2.47	0.50
2:L:115:VAL:O	2:L:207:LYS:HE3	2.10	0.50
2:L:159:SER:HA	2:L:178:THR:O	2.11	0.50
2:M:28(A):ILE:HD13	2:M:71:PHE:CE2	2.43	0.50
1:H:266:ILE:HD13	1:H:266:ILE:O	2.12	0.50
1:H:314:ASN:OD1	3:H:479:NAG:C1	2.59	0.50
1:H:100(J):MET:N	1:H:100(J):MET:SD	2.83	0.50
1:H:235:LYS:O	1:H:236:THR:C	2.50	0.50
1:H:27:TYR:HB2	1:H:28:ARG:NH2	2.13	0.50
1:H:258:PRO:HD2	1:H:332:TRP:CH2	2.47	0.50
1:H:464:HIS:O	1:H:465:ASN:HB2	2.11	0.50
1:K:14:PRO:HD3	1:K:112:SER:O	2.12	0.50
1:K:40:ALA:HA	1:K:88:ALA:HB2	1.92	0.50
2:M:134:CYS:HB2	2:M:148:TRP:CH2	2.47	0.50
2:M:188:LYS:N	2:M:211:ARG:NH1	2.51	0.50
2:M:28(A):ILE:N	2:M:28(A):ILE:HD12	2.26	0.50
1:H:266:ILE:HD13	1:H:266:ILE:C	2.32	0.50
1:K:120:SER:HB3	1:K:122:PHE:CZ	2.47	0.50
1:K:72:ASP:HB3	1:K:75:ALA:HB3	1.94	0.49
1:H:211:ASN:ND2	1:H:218:LYS:HE2	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:59:SER:OG	2:M:61:ARG:HG3	2.11	0.49
1:H:163:SER:HA	1:H:209:ASN:ND2	2.28	0.49
1:H:324:VAL:HG23	1:H:324:VAL:O	2.12	0.49
1:K:193:VAL:HG11	1:K:206:TYR:OH	2.12	0.49
2:L:2:ILE:N	2:L:2:ILE:HD12	2.27	0.49
2:M:165:GLU:O	2:M:166:GLN:C	2.49	0.49
2:M:198:HIS:CD2	2:M:200:GLY:H	2.30	0.49
1:H:344:ASN:HD22	1:H:345:LYS:H	1.60	0.49
1:K:339:LYS:CB	1:K:354:THR:HG22	2.42	0.49
2:L:19:ALA:HB3	2:L:75:ILE:CG1	2.39	0.49
1:H:35:HIS:CD2	1:H:47:TRP:NE1	2.77	0.49
1:H:54:ASN:OD1	1:H:56:ASN:ND2	2.43	0.49
1:H:157:TRP:CZ3	1:H:208:CYS:HB3	2.48	0.49
1:H:19:LYS:HE2	1:H:79:TYR:HD2	1.78	0.49
1:H:40:ALA:HA	1:H:88:ALA:CB	2.43	0.49
1:H:193:VAL:HG22	1:H:194:PRO:CD	2.41	0.49
2:L:89:GLN:NE2	2:L:91:TYR:HB3	2.27	0.49
1:H:4:LEU:CD1	1:H:24:ALA:HB2	2.43	0.49
2:M:47:VAL:HG12	2:M:48:ILE:HG12	1.94	0.49
1:K:208:CYS:C	1:K:209:ASN:HD22	2.16	0.48
1:K:52:ASN:HB3	1:K:54:ASN:ND2	2.28	0.48
2:L:13:LEU:N	2:L:13:LEU:HD12	2.28	0.48
1:H:150:GLU:HB2	1:H:151:PRO:CA	2.33	0.48
1:H:391:LEU:HD12	1:H:392:VAL:N	2.28	0.48
2:L:135:LEU:C	2:L:136:LEU:HD12	2.33	0.48
2:L:198:HIS:CD2	2:L:200:GLY:H	2.31	0.48
1:H:10:GLU:HB3	1:H:12:LYS:NZ	2.29	0.48
2:M:25:SER:OG	2:M:28(A):ILE:HD11	2.13	0.48
1:K:52:ASN:ND2	1:K:53:TYR:HB3	2.28	0.48
2:M:83:PHE:CE2	2:M:106:ARG:HA	2.49	0.48
2:M:150:VAL:HG13	2:M:192:TYR:HE1	1.79	0.48
1:K:122:PHE:O	1:K:143:LEU:HB3	2.14	0.48
1:K:221:LYS:HE3	1:K:221:LYS:CA	2.26	0.48
2:L:120:PRO:HD2	2:L:186:TYR:OH	2.14	0.48
1:H:401:ALA:HB3	1:H:459:MET:HB2	1.95	0.48
1:K:141:GLY:HA2	1:K:157:TRP:HH2	1.78	0.48
1:K:56:ASN:C	1:K:57:LYS:HG3	2.34	0.48
1:H:440:LYS:HE2	8:H:491:HOH:O	2.12	0.48
2:M:183:LYS:HA	2:M:186:TYR:HB3	1.96	0.48
1:K:140:LEU:HD12	1:K:140:LEU:O	2.14	0.48
2:L:150:VAL:O	2:L:151:ASP:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:87:THR:O	1:H:88:ALA:HB2	2.14	0.48
1:K:28:ARG:CG	1:K:31:ASN:HB2	2.44	0.48
1:K:40:ALA:HB3	1:K:43:GLN:HG3	1.94	0.48
1:H:275:VAL:HG23	1:H:322:VAL:HG22	1.95	0.47
1:H:59:PHE:HD2	1:H:64:GLN:HA	1.77	0.47
1:K:35:HIS:CE1	1:K:100(J):MET:HE1	2.48	0.47
1:K:123:PRO:HD3	1:K:221:LYS:HG2	1.95	0.47
1:H:339:LYS:HG2	1:H:354:THR:CG2	2.38	0.47
1:K:140:LEU:HD11	1:K:206:TYR:CD1	2.49	0.47
1:K:209:ASN:HD22	1:K:209:ASN:N	2.11	0.47
2:L:119:PRO:HB3	2:L:209:PHE:CE2	2.49	0.47
1:H:314:ASN:O	1:H:317:SER:HB3	2.15	0.47
2:L:21:PHE:O	2:L:72:THR:HG23	2.14	0.47
1:K:251:PRO:HD2	1:K:347:LEU:CD2	2.44	0.47
2:L:163:VAL:CG1	2:L:164:THR:N	2.78	0.47
2:M:150:VAL:HG13	2:M:192:TYR:CE1	2.50	0.47
1:H:248:LEU:C	1:H:250:GLY:H	2.18	0.47
2:L:36:TYR:HE1	2:L:89:GLN:HG2	1.79	0.47
1:H:147:TYR:CE2	1:H:152:VAL:HG13	2.49	0.47
2:L:72:THR:HG22	2:L:73:LEU:H	1.79	0.47
2:L:113:PRO:HB3	2:L:139:PHE:HB3	1.97	0.47
2:L:4:LEU:HD23	2:L:25:SER:CB	2.45	0.47
1:K:213:LYS:HB2	1:K:214:PRO:HD3	1.96	0.47
1:K:367:PRO:HG2	1:K:463:LEU:HD21	1.97	0.47
1:K:70:THR:OG1	1:K:79:TYR:HB2	2.15	0.47
2:L:2:ILE:HD12	2:L:2:ILE:H	1.80	0.47
1:H:140:LEU:C	1:H:140:LEU:HD12	2.36	0.46
1:H:312:GLN:NE2	1:H:320:ARG:HB2	2.29	0.46
1:H:54:ASN:OD1	1:H:56:ASN:HB2	2.14	0.46
1:H:241:PRO:O	1:H:242:CYS:SG	2.71	0.46
1:H:339:LYS:HE2	1:H:354:THR:CG2	2.45	0.46
1:K:314:ASN:OD1	3:K:479:NAG:C1	2.63	0.46
1:K:291:TYR:CD1	1:K:339:LYS:HD2	2.50	0.46
1:H:230:CYS:O	2:L:214:CYS:SG	2.73	0.46
1:H:100(B):ASP:HB2	1:H:100(F):ASP:CB	2.45	0.46
1:H:124:LEU:HD12	1:H:124:LEU:N	2.30	0.46
1:K:10:GLU:HG3	1:K:18:VAL:HG23	1.96	0.46
1:K:474:LEU:HG	1:K:475:SER:N	2.30	0.46
2:L:165:GLU:O	2:L:166:GLN:C	2.55	0.46
1:H:336:LYS:HB3	1:H:338:TYR:CE1	2.51	0.46
1:H:475:SER:O	1:H:476:PRO:C	2.53	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:58:ILE:HD12	2:L:58:ILE:N	2.31	0.46
2:L:59:SER:C	2:L:61:ARG:N	2.69	0.46
2:M:144:ALA:C	2:M:145:LYS:HG3	2.35	0.46
1:H:216:ASN:HD22	1:H:216:ASN:HA	1.53	0.46
2:M:146:VAL:HG13	2:M:146:VAL:O	2.16	0.46
1:H:82:LEU:HD13	1:H:82(A):ARG:H	1.80	0.45
1:K:52:ASN:HD22	1:K:53:TYR:H	1.64	0.45
1:H:338:TYR:O	1:H:354:THR:HA	2.16	0.45
1:K:32:PHE:O	1:K:34:ILE:HD12	2.16	0.45
2:M:120:PRO:HD3	2:M:132:VAL:HG22	1.99	0.45
2:M:155:GLN:NE2	2:M:179:LEU:HD11	2.31	0.45
1:K:230:CYS:O	1:K:232:ASP:HB2	2.16	0.45
2:L:106:ARG:HG2	2:L:171:SER:OG	2.15	0.45
1:H:50:TRP:O	1:H:57:LYS:HA	2.16	0.45
1:K:261:LYS:HE3	1:K:459:MET:HE1	1.98	0.45
1:K:51:ILE:HG13	1:K:57:LYS:HG2	1.99	0.45
2:M:124:GLN:NE2	2:M:131:SER:H	2.14	0.45
2:M:21:PHE:HB3	8:M:218:HOH:O	2.15	0.45
1:K:251:PRO:HD2	1:K:347:LEU:HD21	1.98	0.45
1:K:307:LYS:HE3	1:K:324:VAL:CG2	2.47	0.45
2:L:48:ILE:HG23	2:L:53:ASN:H	1.81	0.45
1:H:10:GLU:HB3	1:H:12:LYS:HZ2	1.81	0.45
2:L:163:VAL:HG12	2:L:164:THR:N	2.31	0.45
1:H:150:GLU:HG2	1:H:185:TYR:CE2	2.52	0.45
1:H:367:PRO:HG2	1:H:463:LEU:HD21	1.98	0.45
1:K:146:ASP:HB3	1:K:184:LEU:HD13	1.99	0.45
1:K:390:CYS:HB2	1:K:406:TRP:CZ2	2.52	0.45
2:L:48:ILE:HD13	2:L:54:ARG:HA	1.98	0.45
1:H:240:PRO:HA	1:H:241:PRO:HD3	1.69	0.45
1:K:126:PRO:HD2	1:K:227:PRO:HA	1.99	0.45
2:L:8:PRO:O	2:L:102:THR:HG23	2.16	0.45
1:H:197:SER:HA	1:H:200:THR:OG1	2.17	0.44
1:H:256:PHE:HE1	1:H:275:VAL:CG1	2.30	0.44
1:H:51:ILE:HD13	1:H:52:ASN:C	2.37	0.44
2:M:129:THR:HA	2:M:182:SER:HA	1.99	0.44
2:M:125:LEU:C	2:M:183:LYS:HD2	2.37	0.44
2:M:4:LEU:HD11	2:M:90:VAL:HG23	1.98	0.44
1:H:100:TRP:CE3	1:H:100(A):ASP:HB3	2.52	0.44
1:H:184:LEU:N	1:H:184:LEU:HD22	2.33	0.44
1:H:163:SER:CA	1:H:209:ASN:HD21	2.30	0.44
2:L:13:LEU:C	2:L:107:LYS:HB2	2.37	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:50:GLY:O	2:M:51:VAL:HG13	2.18	0.44
2:M:66:GLY:HA3	2:M:71:PHE:HA	1.98	0.44
1:H:100(D):PRO:O	1:H:100(E):GLN:HB2	2.18	0.44
1:H:154:VAL:HG11	1:H:189:SER:CB	2.48	0.44
1:H:449:GLN:HA	1:H:474:LEU:HD22	1.99	0.44
1:K:193:VAL:HG11	1:K:206:TYR:CE1	2.53	0.44
1:H:133:THR:O	1:H:135:GLY:N	2.51	0.44
1:K:124:LEU:HB3	2:M:118:PHE:CD1	2.52	0.44
1:K:52:ASN:HD21	1:K:53:TYR:HB3	1.82	0.44
1:K:67:VAL:HA	1:K:81:GLU:O	2.18	0.44
2:L:150:VAL:HG12	2:L:189:HIS:CD2	2.53	0.44
2:M:187:GLU:HA	2:M:211:ARG:NH2	2.33	0.44
1:K:54:ASN:HD22	1:K:55:GLY:N	2.16	0.44
2:L:135:LEU:HD12	2:L:136:LEU:H	1.83	0.44
2:M:159:SER:HB3	2:M:179:LEU:CD1	2.48	0.44
2:M:198:HIS:CG	2:M:199:GLN:H	2.35	0.44
1:H:163:SER:HA	1:H:209:ASN:HD21	1.83	0.44
1:H:261:LYS:HE2	8:H:496:HOH:O	2.16	0.44
1:K:139:ALA:HB3	2:M:116:PHE:CD1	2.53	0.44
1:K:320:ARG:HE	3:K:480:NAG:H81	1.81	0.44
2:M:107:LYS:HA	2:M:140:TYR:OH	2.17	0.44
1:H:63:PHE:HB3	1:H:67:VAL:HG21	1.99	0.43
2:M:1:GLU:CG	2:M:2:ILE:H	2.04	0.43
1:K:307:LYS:HE3	1:K:324:VAL:HG21	2.01	0.43
1:H:273:THR:HG23	1:H:322:VAL:CG1	2.48	0.43
1:K:156:SER:HB2	1:K:209:ASN:HB2	2.00	0.43
1:K:307:LYS:HB3	1:K:308:PRO:HD2	1.99	0.43
1:K:437:LEU:C	1:K:437:LEU:HD12	2.37	0.43
1:K:62:LYS:HB2	1:K:63:PHE:CD1	2.54	0.43
2:L:120:PRO:HD2	2:L:186:TYR:CZ	2.53	0.43
1:K:177:VAL:HG22	1:K:186:SER:O	2.18	0.43
1:K:445:LYS:O	1:K:449:GLN:HG2	2.18	0.43
2:M:159:SER:HB3	2:M:179:LEU:HD12	2.00	0.43
2:M:50:GLY:C	2:M:51:VAL:HG13	2.39	0.43
1:H:312:GLN:HB2	1:H:318:THR:OG1	2.19	0.43
1:K:474:LEU:O	1:K:475:SER:HB3	2.18	0.43
1:K:75:ALA:CB	1:K:77:THR:HG22	2.49	0.43
2:M:170:ASP:OD2	2:M:172:THR:OG1	2.36	0.43
2:M:198:HIS:CG	2:M:199:GLN:N	2.85	0.43
1:K:397:PRO:O	1:K:460:HIS:HE1	2.02	0.43
2:L:50:GLY:O	2:L:51:VAL:HB	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:30:SER:OG	1:H:53:TYR:HA	2.19	0.43
1:H:343:SER:OG	1:H:350:PRO:HB3	2.19	0.43
1:H:9:ALA:C	1:H:10:GLU:HG3	2.39	0.43
1:K:39:GLN:O	1:K:88:ALA:HB1	2.18	0.43
2:M:155:GLN:CG	2:M:158:ASN:HD21	2.32	0.43
1:H:121:VAL:HG23	1:H:121:VAL:O	2.19	0.43
1:H:325:LEU:O	1:H:327:VAL:HG13	2.18	0.43
1:H:445:LYS:O	1:H:449:GLN:HG3	2.19	0.43
1:H:66:ARG:NH2	1:H:82:LEU:HD11	2.26	0.43
1:K:207:ILE:HG12	1:K:222:LYS:HG2	1.99	0.43
1:K:52:ASN:C	1:K:52:ASN:ND2	2.72	0.43
1:H:117:LYS:CG	1:H:118:GLY:N	2.81	0.43
1:H:120:SER:O	1:H:144:VAL:HA	2.19	0.43
1:H:239:CYS:HA	1:H:240:PRO:HD2	1.71	0.43
1:H:33:VAL:HB	1:H:95:VAL:HG23	1.99	0.43
1:H:348:PRO:HB3	2:M:202:ARG:HB3	2.00	0.43
1:H:95:VAL:HG13	1:H:100(H):TYR:HA	2.00	0.43
1:K:207:ILE:CG1	1:K:222:LYS:HG2	2.48	0.43
1:K:464:HIS:O	1:K:465:ASN:HB2	2.19	0.43
2:M:187:GLU:HA	2:M:211:ARG:NH1	2.33	0.43
1:H:172:HIS:HE1	2:L:138:ASN:OD1	2.02	0.43
1:H:33:VAL:HG13	1:H:51:ILE:O	2.19	0.43
2:M:115:VAL:C	2:M:116:PHE:HD2	2.23	0.42
2:M:180:THR:O	2:M:181:LEU:HD22	2.18	0.42
2:M:35:TRP:CD2	2:M:73:LEU:HB2	2.54	0.42
1:H:364:PRO:HA	1:H:396:TYR:O	2.19	0.42
2:L:31:ARG:O	2:L:51:VAL:HG23	2.18	0.42
1:H:51:ILE:C	1:H:51:ILE:HD13	2.40	0.42
2:L:148:TRP:CG	2:L:179:LEU:HD23	2.55	0.42
2:M:179:LEU:HD12	2:M:179:LEU:HA	1.88	0.42
1:H:284:PRO:HB3	1:H:319:TYR:CE2	2.55	0.42
1:K:14:PRO:HD3	1:K:112:SER:C	2.39	0.42
1:K:314:ASN:CG	3:K:479:NAG:C1	2.88	0.42
2:M:118:PHE:HA	2:M:119:PRO:HD3	1.77	0.42
1:H:211:ASN:HD21	1:H:218:LYS:HE2	1.83	0.42
2:M:155:GLN:HE21	2:M:158:ASN:HD21	1.64	0.42
2:L:175:LEU:HD23	2:L:175:LEU:C	2.39	0.42
2:M:29:ARG:HD3	2:M:29:ARG:HA	1.85	0.42
1:H:344:ASN:HD22	1:H:345:LYS:N	2.18	0.42
1:H:121:VAL:HG11	1:H:219:VAL:CG1	2.50	0.42
1:H:148:PHE:CE2	1:H:149:PRO:HB3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:125:ALA:HA	1:K:126:PRO:HD3	1.89	0.41
1:H:269:THR:HA	1:H:270:PRO:HD3	1.83	0.41
1:H:388:LEU:HD13	1:H:472:LEU:HD23	2.01	0.41
1:H:38:ARG:HB3	1:H:90:TYR:CD2	2.55	0.41
1:H:9:ALA:O	1:H:10:GLU:HG3	2.20	0.41
2:M:155:GLN:CG	2:M:156:SER:N	2.83	0.41
2:M:208:SER:OG	2:M:209:PHE:N	2.53	0.41
2:L:20:THR:HG22	2:L:74:THR:HG22	2.03	0.41
1:H:32:PHE:O	1:H:52(A):PRO:HD2	2.21	0.41
1:H:36:TRP:CE3	1:H:80:MET:HB2	2.56	0.41
1:K:291:TYR:HB2	1:K:339:LYS:HB3	2.03	0.41
1:H:119:PRO:HA	1:H:147:TYR:HB3	2.01	0.41
1:H:274:CYS:HB2	1:H:290:TRP:CH2	2.56	0.41
1:K:421:THR:HA	1:K:439:SER:HA	2.02	0.41
2:L:133:VAL:HG12	2:L:134:CYS:N	2.34	0.41
1:H:331:ASP:HB3	1:H:338:TYR:OH	2.21	0.41
1:H:57:LYS:HG2	1:H:59:PHE:HE1	1.86	0.41
1:K:119:PRO:HD2	1:K:217:THR:CG2	2.48	0.41
1:H:2:VAL:HG23	1:H:2:VAL:O	2.21	0.41
2:M:124:GLN:HE21	2:M:130:ALA:HA	1.86	0.41
1:H:174:PHE:HA	1:H:175:PRO:HD3	1.90	0.41
1:H:253:VAL:HB	1:H:351:ILE:HG21	2.02	0.41
1:H:67:VAL:CG1	1:H:68:THR:N	2.84	0.41
1:K:54:ASN:ND2	1:K:54:ASN:C	2.73	0.41
1:H:123:PRO:HG3	1:H:221:LYS:HD3	2.03	0.41
1:H:369:VAL:HG21	1:H:468:THR:CG2	2.51	0.41
1:H:4:LEU:HG	1:H:22:CYS:SG	2.60	0.41
2:M:61:ARG:CZ	2:M:79:GLU:HG2	2.51	0.41
1:K:54:ASN:ND2	1:K:56:ASN:HB2	2.33	0.40
2:L:25:SER:OG	2:L:27:HIS:O	2.32	0.40
2:M:14:SER:O	2:M:15:PRO:C	2.60	0.40
1:H:363:GLN:O	1:H:396:TYR:HD2	2.04	0.40
1:H:242:CYS:O	1:H:242:CYS:SG	2.79	0.40
1:H:18:VAL:HG23	1:H:82(C):LEU:CD1	2.52	0.40
1:K:338:TYR:O	1:K:354:THR:HA	2.21	0.40
3:K:483:NAG:HO3	3:K:483:NAG:C7	2.33	0.40
1:H:121:VAL:HG21	1:H:219:VAL:CG1	2.38	0.40
1:H:27:TYR:CE2	1:H:94:ARG:HD3	2.56	0.40
1:H:94:ARG:O	1:H:101:ASP:HB3	2.22	0.40
1:K:253:VAL:HG22	1:K:342:VAL:HG21	2.03	0.40
1:K:40:ALA:HA	1:K:88:ALA:CB	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:115:VAL:C	2:M:116:PHE:CD2	2.95	0.40
2:M:50:GLY:O	2:M:52:SER:N	2.50	0.40
1:H:266:ILE:O	1:H:268:ARG:N	2.55	0.40
1:K:10:GLU:OE1	1:K:12:LYS:NZ	2.55	0.40
1:K:148:PHE:CE2	1:K:149:PRO:HB3	2.56	0.40
1:K:239:CYS:O	1:K:241:PRO:HD3	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:136:GLY:CA	1:H:136:GLY:CA[4_557]	1.86	0.34

## 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	H	455/457 (100%)	400 (88%)	48 (10%)	7 (2%)	12	30
1	K	438/457 (96%)	402 (92%)	30 (7%)	6 (1%)	13	33
2	L	213/215 (99%)	193 (91%)	17 (8%)	3 (1%)	13	33
2	M	213/215 (99%)	195 (92%)	15 (7%)	3 (1%)	13	33
All	All	1319/1344 (98%)	1190 (90%)	110 (8%)	19 (1%)	13	33

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	99	SER
1	H	239	CYS
1	H	476	PRO
1	H	477	GLY

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Mol	Chain	Res	Type
1	K	16	ALA
1	K	146	ASP
1	K	191	VAL
2	L	154	LEU
2	M	51	VAL
2	M	157	GLY
1	H	267	SER
1	K	29	PHE
1	K	232	ASP
1	K	241	PRO
1	H	134	SER
2	L	212	GLY
2	M	162	SER
1	H	14	PRO
2	L	68	GLY

### 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	H	405/405 (100%)	376 (93%)	29 (7%)	17	39
1	K	395/405 (98%)	378 (96%)	17 (4%)	33	64
2	L	187/187 (100%)	179 (96%)	8 (4%)	33	64
2	M	187/187 (100%)	171 (91%)	16 (9%)	12	28
All	All	1174/1184 (99%)	1104 (94%)	70 (6%)	22	48

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	28	ARG
1	H	38	ARG
1	H	51	ILE
1	H	57	LYS
1	H	80	MET
1	H	82	LEU

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Mol	Chain	Res	Type
1	H	82(A)	ARG
1	H	100(J)	MET
1	H	108	THR
1	H	153	THR
1	H	166	LEU
1	H	216	ASN
1	H	237	HIS
1	H	238	THR
1	H	239	CYS
1	H	262	ASP
1	H	266	ILE
1	H	269	THR
1	H	311	GLU
1	H	313	TYR
1	H	330	GLN
1	H	344	ASN
1	H	347	LEU
1	H	400	ILE
1	H	418	ASN
1	H	437	LEU
1	H	457	SER
1	H	469	GLN
1	H	476	PRO
1	K	4	LEU
1	K	28	ARG
1	K	31	ASN
1	K	38	ARG
1	K	52	ASN
1	K	54	ASN
1	K	94	ARG
1	K	100(J)	MET
1	K	107	THR
1	K	187	LEU
1	K	221	LYS
1	K	239	CYS
1	K	246	GLU
1	K	271	GLU
1	K	365	ARG
1	K	400	ILE
1	K	418	ASN
2	L	13	LEU
2	L	76	THR

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Mol	Chain	Res	Type
2	L	95	SER
2	L	104	LEU
2	L	107	LYS
2	L	108	ARG
2	L	142	ARG
2	L	179	LEU
2	M	27	HIS
2	M	51	VAL
2	M	60	ASP
2	M	63	SER
2	M	69	THR
2	M	74	THR
2	M	81	GLU
2	M	100	GLN
2	M	105	GLU
2	M	108	ARG
2	M	122	ASP
2	M	143	GLU
2	M	170	ASP
2	M	181	LEU
2	M	202	ARG
2	M	206	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	3	GLN
1	H	31	ASN
1	H	35	HIS
1	H	56	ASN
1	H	76	ASN
1	H	162	ASN
1	H	172	HIS
1	H	179	GLN
1	H	209	ASN
1	H	216	ASN
1	H	312	GLN
1	H	329	HIS
1	H	344	ASN
1	H	368	GLN
1	H	384	ASN
1	H	418	ASN

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Mol	Chain	Res	Type
1	H	452	ASN
1	H	460	HIS
1	H	466	HIS
1	K	31	ASN
1	K	35	HIS
1	K	52	ASN
1	K	54	ASN
1	K	172	HIS
1	K	314	ASN
1	K	368	GLN
1	K	418	ASN
1	K	450	GLN
1	K	452	ASN
1	K	460	HIS
1	K	465	ASN
1	K	466	HIS
2	L	42	GLN
2	L	89	GLN
2	L	137	ASN
2	L	147	GLN
2	L	152	ASN
2	L	198	HIS
2	M	100	GLN
2	M	124	GLN
2	M	137	ASN
2	M	158	ASN
2	M	198	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

18 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$
3	NAG	H	479	3	14,14,15	0.44	0	15,19,21	0.95	0
3	NAG	H	480	3,4	14,14,15	0.36	0	15,19,21	0.89	1 (6%)
4	BMA	H	481	3,5	11,11,12	0.50	0	13,15,17	0.92	1 (7%)
5	MAN	H	482	3,4	11,11,12	0.56	0	13,15,17	0.76	0
3	NAG	H	483	5,6	14,14,15	0.64	0	15,19,21	0.87	1 (6%)
6	GAL	H	484	3	11,11,12	0.45	0	13,15,17	0.42	0
5	MAN	H	485	3,4	11,11,12	0.71	0	13,15,17	0.61	0
3	NAG	H	486	5,6	14,14,15	0.63	0	15,19,21	1.08	2 (13%)
6	GAL	H	487	3	11,11,12	0.56	0	13,15,17	0.35	0
3	NAG	K	479	3,7	14,14,15	0.42	0	15,19,21	1.05	1 (6%)
3	NAG	K	480	3,4	14,14,15	0.49	0	15,19,21	0.90	1 (6%)
4	BMA	K	481	3,5	11,11,12	0.69	0	13,15,17	0.66	0
5	MAN	K	482	3,4	11,11,12	0.57	0	13,15,17	1.16	1 (7%)
3	NAG	K	483	5	14,14,15	0.56	0	15,19,21	0.72	0
5	MAN	K	484	3,4	11,11,12	0.82	0	13,15,17	0.62	0
3	NAG	K	485	5,6	14,14,15	0.52	0	15,19,21	1.08	1 (6%)
6	GAL	K	486	3	11,11,12	0.54	0	13,15,17	0.40	0
7	FUC	K	487	3	9,10,11	0.63	0	13,14,16	0.45	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
3	NAG	H	479	3	-	0/6/23/26	0/1/1/1
3	NAG	H	480	3,4	-	0/6/23/26	0/1/1/1
4	BMA	H	481	3,5	-	0/2/19/22	0/1/1/1
5	MAN	H	482	3,4	-	0/2/19/22	0/1/1/1
3	NAG	H	483	5,6	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GAL	H	484	3	-	0/2/19/22	0/1/1/1
5	MAN	H	485	3,4	-	0/2/19/22	0/1/1/1
3	NAG	H	486	5,6	-	0/6/23/26	0/1/1/1
6	GAL	H	487	3	-	0/2/19/22	0/1/1/1
3	NAG	K	479	3,7	-	0/6/23/26	0/1/1/1
3	NAG	K	480	3,4	-	0/6/23/26	0/1/1/1
4	BMA	K	481	3,5	-	0/2/19/22	0/1/1/1
5	MAN	K	482	3,4	-	0/2/19/22	0/1/1/1
3	NAG	K	483	5	-	0/6/23/26	0/1/1/1
5	MAN	K	484	3,4	-	0/2/19/22	0/1/1/1
3	NAG	K	485	5,6	-	0/6/23/26	0/1/1/1
6	GAL	K	486	3	-	0/2/19/22	0/1/1/1
7	FUC	K	487	3	-	0/0/17/20	0/1/1/1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	486	NAG	C2-N2-C7	-2.83	118.82	122.94
3	K	485	NAG	C2-N2-C7	-2.71	119.00	122.94
3	K	479	NAG	C2-N2-C7	-2.68	119.03	122.94
3	K	480	NAG	C2-N2-C7	-2.50	119.30	122.94
3	H	480	NAG	C2-N2-C7	-2.45	119.36	122.94
4	H	481	BMA	O3-C3-C2	-2.29	105.86	110.02
3	H	486	NAG	O5-C1-C2	-2.16	108.47	111.47
3	H	483	NAG	C2-N2-C7	-2.13	119.84	122.94
5	K	482	MAN	C1-O5-C5	2.46	115.56	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	479	NAG	5	0
3	H	480	NAG	1	0
3	H	483	NAG	3	0
6	H	484	GAL	3	0
3	H	486	NAG	2	0
3	K	479	NAG	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	K	480	NAG	2	0
3	K	483	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 ⓘ

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	H	457/457 (100%)	0.63	55 (12%) 5 4	29, 97, 181, 199	0
1	K	444/457 (97%)	0.23	37 (8%) 12 9	28, 67, 159, 197	0
2	L	215/215 (100%)	0.05	9 (4%) 37 35	43, 89, 146, 164	0
2	M	215/215 (100%)	0.19	17 (7%) 13 11	36, 77, 167, 193	0
All	All	1331/1344 (99%)	0.33	118 (8%) 10 8	28, 83, 167, 199	0

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	235	LYS	11.7
1	K	242	CYS	9.9
1	H	236	THR	7.5
1	H	241	PRO	7.5
1	H	238	THR	7.3
1	K	232	ASP	7.1
1	H	239	CYS	6.9
1	H	240	PRO	6.9
1	K	241	PRO	6.8
1	K	248	LEU	6.8
1	K	244	ALA	6.6
1	H	478	LYS	6.5
1	K	239	CYS	6.4
1	H	319	TYR	6.3
1	K	246	GLU	6.2
1	H	287	LYS	6.0
2	M	119	PRO	5.9
1	H	242	CYS	5.8
1	K	124	LEU	5.7
2	M	118	PHE	5.6
1	H	243	PRO	5.4

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Mol	Chain	Res	Type	RSRZ
1	H	247	LEU	5.4
1	H	134	SER	5.3
1	K	141	GLY	5.3
1	H	130	SER	5.2
1	K	240	PRO	5.2
1	K	125	ALA	5.1
1	K	229	SER	4.9
1	H	313	TYR	4.9
1	H	265	MET	4.8
1	K	142	CYS	4.7
1	H	320	ARG	4.6
1	K	243	PRO	4.5
1	H	296	GLY	4.4
1	H	349	ALA	4.4
1	K	245	PRO	4.2
1	H	235	LYS	4.2
1	H	284	PRO	4.2
1	H	232	ASP	4.2
1	H	114	ALA	4.1
1	H	237	HIS	4.1
1	H	248	LEU	4.1
1	H	477	GLY	4.1
1	K	230	CYS	3.9
1	K	228	LYS	3.9
1	K	165	ALA	3.7
1	H	317	SER	3.6
1	H	264	LEU	3.6
1	H	230	CYS	3.5
1	K	123	PRO	3.5
2	M	202	ARG	3.5
1	K	166	LEU	3.4
1	K	313	TYR	3.4
1	K	164	GLY	3.4
1	H	291	TYR	3.3
1	H	288	PHE	3.3
1	H	1	GLN	3.2
1	K	227	PRO	3.2
2	M	149	LYS	3.1
2	M	188	LYS	3.1
2	L	118	PHE	3.1
1	H	249	GLY	3.1
2	M	190	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	H	245	PRO	3.1
1	H	92	CYS	3.0
1	H	35	HIS	3.0
1	H	113	SER	3.0
1	K	222	LYS	3.0
1	K	92	CYS	3.0
2	M	154	LEU	3.0
1	H	37	VAL	2.9
1	H	346	ALA	2.9
1	K	200	THR	2.9
2	L	190	LYS	2.9
1	K	198	LEU	2.9
1	H	295	ASP	2.9
1	H	300	GLU	2.8
2	M	121	SER	2.8
1	K	197	SER	2.8
1	K	225	ALA	2.8
2	L	152	ASN	2.8
1	H	286	VAL	2.8
2	L	211	ARG	2.8
2	M	117	ILE	2.7
1	H	285	GLU	2.7
1	H	299	VAL	2.7
2	L	134	CYS	2.7
1	K	100(J)	MET	2.6
1	H	321	VAL	2.6
2	M	153	ALA	2.5
2	M	150	VAL	2.5
1	K	218	LYS	2.5
1	H	345	LYS	2.5
2	L	187	GLU	2.4
2	M	183	LYS	2.4
1	H	36	TRP	2.4
1	K	122	PHE	2.4
2	M	213	GLU	2.4
2	M	182	SER	2.4
1	K	140	LEU	2.3
2	M	214	CYS	2.3
1	K	196	SER	2.3
1	H	205	THR	2.3
1	H	342	VAL	2.2
1	H	308	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
2	M	187	GLU	2.2
1	H	125	ALA	2.2
1	H	339	LYS	2.1
2	L	202	ARG	2.1
2	L	133	VAL	2.1
2	L	188	LYS	2.1
1	K	127	SER	2.1
2	M	186	TYR	2.1
1	H	314	ASN	2.1
1	H	93	ALA	2.0
1	H	178	LEU	2.0
1	H	309	ARG	2.0
1	K	193	VAL	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
6	GAL	K	486	11/12	0.58	0.44	8.28	168,168,168,168	0
3	NAG	H	479	14/15	0.74	0.26	-0.39	90,146,146,146	0
3	NAG	K	480	14/15	0.92	0.15	-0.69	84,84,84,84	0
4	BMA	K	481	11/12	0.91	0.10	-	77,77,77,77	0
5	MAN	H	485	11/12	0.82	0.20	-	164,164,164,164	0
3	NAG	H	486	14/15	0.78	0.21	-	136,136,136,136	0
5	MAN	K	482	11/12	0.90	0.16	-	154,154,154,154	0
6	GAL	H	487	11/12	0.77	0.34	-	151,151,151,151	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	H	483	14/15	0.76	0.28	-	172,172,172,172	0
3	NAG	K	485	14/15	0.89	0.16	-	110,110,110,110	0
7	FUC	K	487	10/11	0.78	0.35	-	133,133,133,133	0
6	GAL	H	484	11/12	0.40	0.53	-	198,198,198,198	0
4	BMA	H	481	11/12	0.74	0.15	-	130,130,130,130	0
3	NAG	H	480	14/15	0.70	0.34	-	168,168,168,168	0
3	NAG	K	483	14/15	0.83	0.30	-	157,157,157,157	0
5	MAN	H	482	11/12	0.87	0.28	-	191,191,191,191	0
5	MAN	K	484	11/12	0.92	0.17	-	97,97,97,97	0
3	NAG	K	479	14/15	0.86	0.15	-	95,95,95,95	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.