



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 02:30 PM BST

PDB ID : 1ZS8  
Title : Crystal Structure of the Murine MHC Class Ib Molecule M10.5  
Authors : Olson, R.; Huey-Tubman, K.E.; Dulac, C.; Bjorkman, P.J.  
Deposited on : 2005-07-22  
Resolution : 3.00 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

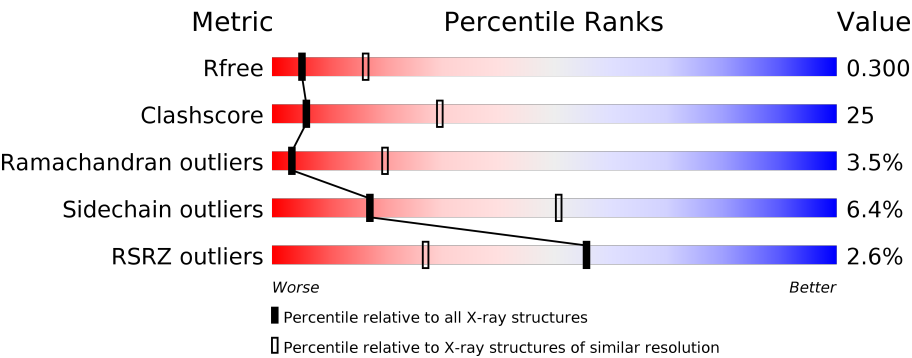
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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  $\leq 5\%$ . 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	274	<div><div>3%</div><div><div></div><div>53%</div><div>36%</div><div>5%</div><div>5%</div></div></div>
1	C	274	<div><div>3%</div><div><div></div><div>54%</div><div>36%</div><div>5%</div><div>5%</div></div></div>
1	E	274	<div><div>3%</div><div><div></div><div>54%</div><div>35%</div><div>5%</div><div>5%</div></div></div>
1	G	274	<div><div>2%</div><div><div></div><div>53%</div><div>36%</div><div>5%</div><div>5%</div></div></div>
1	I	274	<div><div>3%</div><div><div></div><div>53%</div><div>37%</div><div></div><div>5%</div></div></div>
2	B	99	<div><div>%</div><div><div></div><div>68%</div><div>27%</div><div>5%</div></div></div>

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Mol	Chain	Length	Quality of chain
2	D	99	<div> <div>%</div> <div> <div></div> <div>66%</div> <div>29%</div> <div>5%</div> </div> </div>
2	F	99	<div> <div>4%</div> <div> <div></div> <div>65%</div> <div>30%</div> <div>5%</div> </div> </div>
2	H	99	<div> <div></div> <div> <div></div> <div>67%</div> <div>28%</div> <div>5%</div> </div> </div>
2	J	99	<div> <div>2%</div> <div> <div></div> <div>68%</div> <div>27%</div> <div>5%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	C	302	-	-	-	X
3	NAG	E	303	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13735 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 histocompatibility 2, M region locus 10.5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	261	Total	C	N	O	S	0	0	0
			1961	1252	337	362	10			
1	C	261	Total	C	N	O	S	0	0	0
			1961	1252	337	362	10			
1	E	261	Total	C	N	O	S	0	0	0
			1961	1252	337	362	10			
1	G	261	Total	C	N	O	S	0	0	0
			1961	1252	337	362	10			
1	I	261	Total	C	N	O	S	0	0	0
			1961	1252	337	362	10			

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	0	0	0
			772	494	133	142	3			
2	D	99	Total	C	N	O	S	0	0	0
			772	494	133	142	3			
2	F	99	Total	C	N	O	S	0	0	0
			772	494	133	142	3			
2	H	99	Total	C	N	O	S	0	0	0
			772	494	133	142	3			
2	J	99	Total	C	N	O	S	0	0	0
			772	494	133	142	3			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).

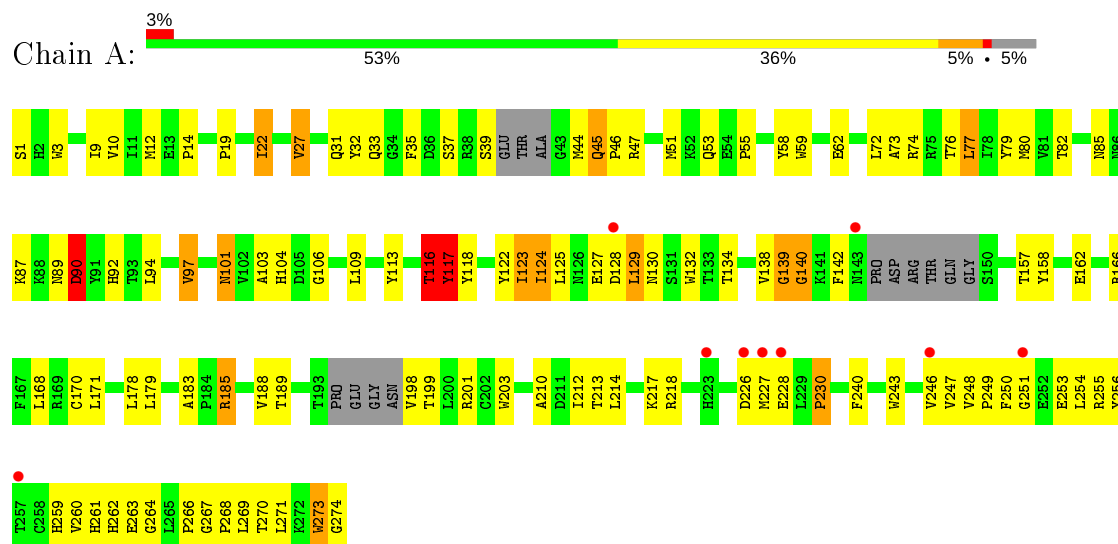


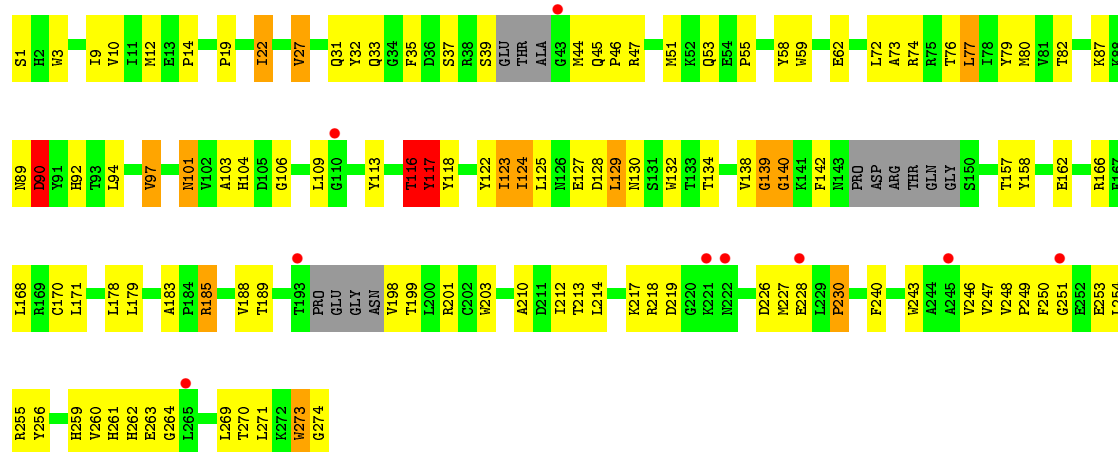
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		
3	G	1	Total	C	N	O	0	0
			14	8	1	5		
3	I	1	Total	C	N	O	0	0
			14	8	1	5		

### 3 Residue-property plots

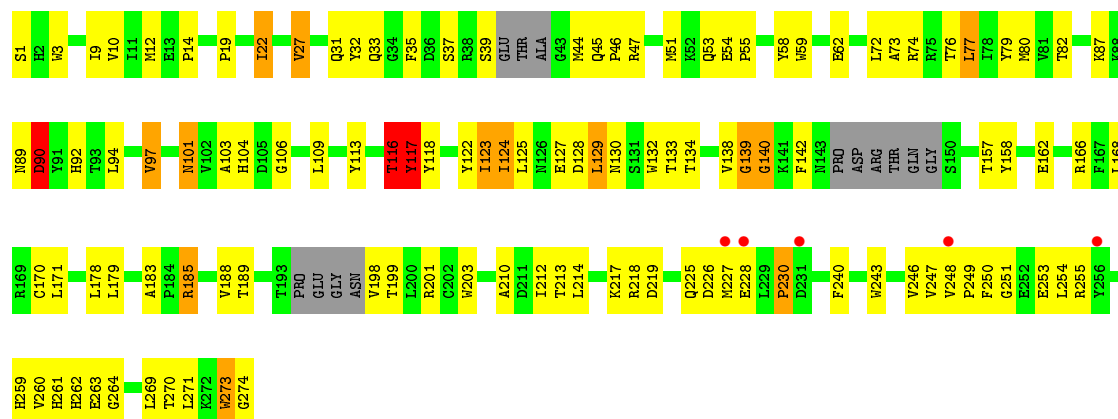
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: histocompatibility 2, M region locus 10.5

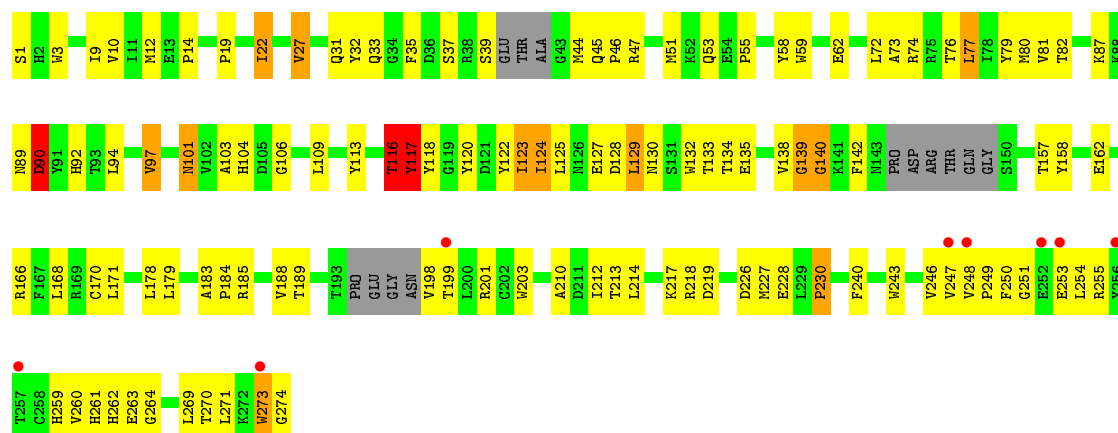




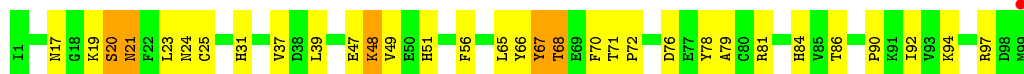
- Molecule 1: histocompatibility 2, M region locus 10.5



- Molecule 1: histocompatibility 2, M region locus 10.5



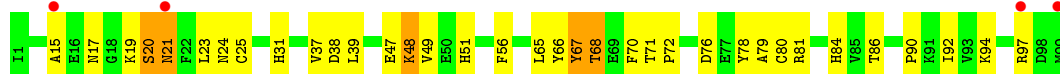
- Molecule 2: Beta-2-microglobulin



• Molecule 2: Beta-2-microglobulin



• Molecule 2: Beta-2-microglobulin



• Molecule 2: Beta-2-microglobulin



• Molecule 2: Beta-2-microglobulin





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	124.11Å 134.71Å 149.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	56.36 – 3.00 56.36 – 2.99	Depositor EDS
% Data completeness (in resolution range)	92.3 (56.36-3.00) 91.3 (56.36-2.99)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	0.16	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.16 (at 3.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.307 , 0.308 0.294 , 0.300	Depositor DCC
$R_{free}$ test set	2355 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	63.0	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 74.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	13735	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

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	0.43	0/2019	0.76	5/2762 (0.2%)
1	C	0.43	0/2019	0.76	5/2762 (0.2%)
1	E	0.43	0/2019	0.76	5/2762 (0.2%)
1	G	0.43	0/2019	0.76	5/2762 (0.2%)
1	I	0.43	0/2019	0.76	5/2762 (0.2%)
2	B	0.44	0/795	0.67	0/1085
2	D	0.44	0/795	0.67	0/1085
2	F	0.44	0/795	0.67	0/1085
2	H	0.44	0/795	0.67	0/1085
2	J	0.44	0/795	0.67	0/1085
All	All	0.43	0/14070	0.73	25/19235 (0.1%)

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	117	TYR	N-CA-C	-8.69	87.53	111.00
1	G	117	TYR	N-CA-C	-8.69	87.53	111.00
1	I	117	TYR	N-CA-C	-8.69	87.53	111.00
1	C	117	TYR	N-CA-C	-8.69	87.54	111.00
1	E	117	TYR	N-CA-C	-8.69	87.55	111.00
1	C	185	ARG	N-CA-C	-6.21	94.24	111.00
1	A	185	ARG	N-CA-C	-6.21	94.25	111.00
1	G	185	ARG	N-CA-C	-6.20	94.25	111.00
1	I	185	ARG	N-CA-C	-6.20	94.26	111.00
1	E	185	ARG	N-CA-C	-6.20	94.27	111.00
1	E	140	GLY	N-CA-C	-5.90	98.36	113.10
1	C	140	GLY	N-CA-C	-5.88	98.41	113.10
1	A	140	GLY	N-CA-C	-5.87	98.43	113.10
1	I	140	GLY	N-CA-C	-5.87	98.44	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	140	GLY	N-CA-C	-5.86	98.45	113.10
1	C	27	VAL	N-CA-C	-5.66	95.73	111.00
1	A	27	VAL	N-CA-C	-5.64	95.77	111.00
1	E	27	VAL	N-CA-C	-5.64	95.77	111.00
1	I	27	VAL	N-CA-C	-5.64	95.78	111.00
1	G	27	VAL	N-CA-C	-5.64	95.78	111.00
1	I	116	THR	CB-CA-C	-5.26	97.40	111.60
1	E	116	THR	CB-CA-C	-5.25	97.42	111.60
1	C	116	THR	CB-CA-C	-5.25	97.43	111.60
1	G	116	THR	CB-CA-C	-5.25	97.43	111.60
1	A	116	THR	CB-CA-C	-5.25	97.44	111.60

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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	1961	0	1730	117	0
1	C	1961	0	1730	105	1
1	E	1961	0	1730	104	1
1	G	1961	0	1730	104	0
1	I	1961	0	1730	121	0
2	B	772	0	694	24	0
2	D	772	0	694	24	0
2	F	772	0	694	24	0
2	H	772	0	694	23	0
2	J	772	0	694	24	0
3	A	14	0	13	2	0
3	C	14	0	13	1	0
3	E	14	0	13	1	0
3	G	14	0	13	1	0
3	I	14	0	13	1	0
All	All	13735	0	12185	641	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 25.

All (641) 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:E:14:PRO:HG3	1:E:90:ASP:HA	1.43	1.00
1:C:14:PRO:HG3	1:C:90:ASP:HA	1.43	1.00
1:G:14:PRO:HG3	1:G:90:ASP:HA	1.42	0.99
1:I:14:PRO:HG3	1:I:90:ASP:HA	1.42	0.97
1:A:14:PRO:HG3	1:A:90:ASP:HA	1.43	0.96
1:G:103:ALA:HB2	1:G:109:LEU:HD21	1.48	0.96
2:H:20:SER:HA	2:H:71:THR:HG22	1.48	0.96
1:A:103:ALA:HB2	1:A:109:LEU:HD21	1.48	0.96
2:F:20:SER:HA	2:F:71:THR:HG22	1.48	0.95
1:E:103:ALA:HB2	1:E:109:LEU:HD21	1.48	0.95
2:D:20:SER:HA	2:D:71:THR:HG22	1.48	0.94
1:I:103:ALA:HB2	1:I:109:LEU:HD21	1.48	0.93
1:C:103:ALA:HB2	1:C:109:LEU:HD21	1.48	0.93
2:J:20:SER:HA	2:J:71:THR:HG22	1.48	0.93
2:B:20:SER:HA	2:B:71:THR:HG22	1.48	0.93
1:G:162:GLU:O	1:G:166:ARG:HG3	1.83	0.78
1:A:162:GLU:O	1:A:166:ARG:HG3	1.83	0.78
1:I:162:GLU:O	1:I:166:ARG:HG3	1.83	0.78
1:C:162:GLU:O	1:C:166:ARG:HG3	1.83	0.77
1:E:162:GLU:O	1:E:166:ARG:HG3	1.83	0.77
1:G:89:ASN:O	1:G:90:ASP:HB3	1.87	0.74
1:I:89:ASN:O	1:I:90:ASP:HB3	1.87	0.74
1:E:89:ASN:O	1:E:90:ASP:HB3	1.87	0.74
1:A:268:PRO:O	1:I:122:TYR:CE1	2.41	0.73
1:A:89:ASN:O	1:A:90:ASP:HB3	1.87	0.73
1:E:10:VAL:HG12	1:E:77:LEU:HD12	1.71	0.73
1:C:89:ASN:O	1:C:90:ASP:HB3	1.87	0.72
1:C:10:VAL:HG12	1:C:77:LEU:HD12	1.71	0.72
1:I:10:VAL:HG12	1:I:77:LEU:HD12	1.71	0.72
1:G:10:VAL:HG12	1:G:77:LEU:HD12	1.71	0.71
1:C:217:LYS:HD2	1:C:259:HIS:HE2	1.56	0.71
1:G:230:PRO:HG2	1:G:243:TRP:CE2	2.26	0.71
1:C:230:PRO:HG2	1:C:243:TRP:CE2	2.26	0.71
1:A:10:VAL:HG12	1:A:77:LEU:HD12	1.71	0.70
1:A:230:PRO:HG2	1:A:243:TRP:CE2	2.26	0.70
1:E:230:PRO:HG2	1:E:243:TRP:CE2	2.26	0.70
1:E:217:LYS:HD2	1:E:259:HIS:HE2	1.56	0.70
1:I:230:PRO:HG2	1:I:243:TRP:CE2	2.26	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:217:LYS:HD2	1:I:259:HIS:HE2	1.56	0.69
1:A:269:LEU:HD21	1:I:135:GLU:OE2	1.93	0.69
1:E:134:THR:HB	1:E:139:GLY:O	1.93	0.68
1:I:134:THR:HB	1:I:139:GLY:O	1.93	0.68
1:A:134:THR:HB	1:A:139:GLY:O	1.93	0.68
1:E:31:GLN:NE2	1:E:47:ARG:HG3	2.09	0.68
1:G:31:GLN:NE2	1:G:47:ARG:HG3	2.09	0.68
1:C:14:PRO:CG	1:C:90:ASP:HA	2.23	0.68
1:C:31:GLN:NE2	1:C:47:ARG:HG3	2.09	0.68
1:E:14:PRO:CG	1:E:90:ASP:HA	2.23	0.67
1:I:31:GLN:NE2	1:I:47:ARG:HG3	2.09	0.67
1:I:103:ALA:HB2	1:I:109:LEU:CD2	2.24	0.67
2:H:72:PRO:HB2	2:H:97:ARG:HH21	1.60	0.67
1:A:31:GLN:NE2	1:A:47:ARG:HG3	2.09	0.67
1:C:134:THR:HB	1:C:139:GLY:O	1.93	0.67
2:J:72:PRO:HB2	2:J:97:ARG:HH21	1.60	0.67
1:E:103:ALA:HB2	1:E:109:LEU:CD2	2.25	0.67
2:B:72:PRO:HB2	2:B:97:ARG:HH21	1.60	0.67
2:F:72:PRO:HB2	2:F:97:ARG:HH21	1.60	0.67
1:G:134:THR:HB	1:G:139:GLY:O	1.94	0.66
1:E:171:LEU:HD11	1:E:179:LEU:HD11	1.77	0.66
1:I:171:LEU:HD11	1:I:179:LEU:HD11	1.77	0.66
1:A:31:GLN:HE21	1:A:47:ARG:HG3	1.61	0.66
1:C:171:LEU:HD11	1:C:179:LEU:HD11	1.77	0.66
2:D:72:PRO:HB2	2:D:97:ARG:HH21	1.60	0.66
1:C:31:GLN:HE21	1:C:47:ARG:HG3	1.61	0.65
1:G:171:LEU:HD11	1:G:179:LEU:HD11	1.77	0.65
1:I:31:GLN:HE21	1:I:47:ARG:HG3	1.61	0.65
1:G:31:GLN:HE21	1:G:47:ARG:HG3	1.60	0.65
1:A:171:LEU:HD11	1:A:179:LEU:HD11	1.77	0.65
1:E:199:THR:HG22	1:E:247:VAL:HG12	1.79	0.65
1:A:199:THR:HG22	1:A:247:VAL:HG12	1.79	0.64
1:G:134:THR:HG22	1:G:142:PHE:HB3	1.79	0.64
1:I:134:THR:HG22	1:I:142:PHE:HB3	1.79	0.64
1:C:134:THR:HG22	1:C:142:PHE:HB3	1.79	0.64
1:G:199:THR:HG22	1:G:247:VAL:HG12	1.79	0.64
1:E:31:GLN:HE21	1:E:47:ARG:HG3	1.61	0.64
1:A:270:THR:HB	1:I:120:TYR:CD1	2.33	0.64
1:A:268:PRO:O	1:I:122:TYR:HE1	1.79	0.64
1:A:266:PRO:HB3	1:I:124:ILE:CD1	2.28	0.64
1:C:199:THR:HG22	1:C:247:VAL:HG12	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:199:THR:HG22	1:I:247:VAL:HG12	1.79	0.64
1:A:217:LYS:HD2	1:A:259:HIS:NE2	2.13	0.63
1:A:134:THR:HG22	1:A:142:PHE:HB3	1.79	0.63
1:C:14:PRO:HG3	1:C:90:ASP:CA	2.26	0.63
1:E:134:THR:HG22	1:E:142:PHE:HB3	1.79	0.63
1:C:217:LYS:HD2	1:C:259:HIS:NE2	2.13	0.63
1:G:217:LYS:HD2	1:G:259:HIS:NE2	2.13	0.63
1:A:103:ALA:HB2	1:A:109:LEU:CD2	2.25	0.63
1:I:14:PRO:CG	1:I:90:ASP:HA	2.23	0.63
1:I:217:LYS:HD2	1:I:259:HIS:NE2	2.13	0.63
1:G:37:SER:C	1:G:39:SER:H	2.03	0.63
2:H:81:ARG:HG3	2:H:92:ILE:HG12	1.81	0.63
2:J:81:ARG:HG3	2:J:92:ILE:HG12	1.81	0.63
1:G:103:ALA:HB2	1:G:109:LEU:CD2	2.25	0.63
2:F:81:ARG:HG3	2:F:92:ILE:HG12	1.81	0.62
2:D:20:SER:CA	2:D:71:THR:HG22	2.28	0.62
1:E:217:LYS:HD2	1:E:259:HIS:NE2	2.13	0.62
2:F:20:SER:CA	2:F:71:THR:HG22	2.28	0.62
1:A:134:THR:HB	1:A:140:GLY:HA2	1.82	0.62
1:A:37:SER:C	1:A:39:SER:H	2.02	0.62
1:I:201:ARG:HD3	1:I:203:TRP:CZ2	2.35	0.62
1:C:201:ARG:HD3	1:C:203:TRP:CZ2	2.35	0.62
1:I:27:VAL:HG13	1:I:27:VAL:O	1.99	0.62
1:C:37:SER:C	1:C:39:SER:H	2.02	0.62
1:G:201:ARG:HD3	1:G:203:TRP:CZ2	2.35	0.62
1:I:37:SER:C	1:I:39:SER:H	2.03	0.62
1:A:201:ARG:HD3	1:A:203:TRP:CZ2	2.35	0.61
1:A:27:VAL:HG13	1:A:27:VAL:O	1.99	0.61
1:E:134:THR:HB	1:E:140:GLY:HA2	1.82	0.61
1:G:134:THR:HB	1:G:140:GLY:HA2	1.82	0.61
1:E:27:VAL:O	1:E:27:VAL:HG13	1.99	0.61
1:A:14:PRO:CG	1:A:90:ASP:HA	2.23	0.61
1:C:103:ALA:HB2	1:C:109:LEU:CD2	2.25	0.61
2:D:81:ARG:HG3	2:D:92:ILE:HG12	1.81	0.61
1:A:203:TRP:CZ3	1:A:243:TRP:HB3	2.36	0.61
1:C:134:THR:HB	1:C:140:GLY:HA2	1.82	0.61
1:E:201:ARG:HD3	1:E:203:TRP:CZ2	2.35	0.61
2:B:81:ARG:HG3	2:B:92:ILE:HG12	1.81	0.61
1:E:123:ILE:C	1:E:124:ILE:HG12	2.21	0.61
1:I:203:TRP:CZ3	1:I:243:TRP:HB3	2.36	0.61
1:I:123:ILE:C	1:I:124:ILE:HG12	2.21	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:ILE:C	1:A:124:ILE:HG12	2.21	0.61
1:G:27:VAL:O	1:G:27:VAL:HG13	1.99	0.61
1:A:267:GLY:HA3	1:I:122:TYR:CE2	2.36	0.61
1:A:266:PRO:HB3	1:I:124:ILE:HD11	1.83	0.61
1:G:203:TRP:CZ3	1:G:243:TRP:HB3	2.36	0.60
1:C:123:ILE:C	1:C:124:ILE:HG12	2.21	0.60
1:G:14:PRO:CG	1:G:90:ASP:HA	2.23	0.60
1:C:27:VAL:HG13	1:C:27:VAL:O	1.99	0.60
2:B:67:TYR:N	2:B:67:TYR:CD1	2.69	0.60
1:G:123:ILE:C	1:G:124:ILE:HG12	2.21	0.60
2:J:67:TYR:CD1	2:J:67:TYR:N	2.69	0.60
1:C:203:TRP:CZ3	1:C:243:TRP:HB3	2.36	0.60
1:E:203:TRP:CZ3	1:E:243:TRP:HB3	2.36	0.60
1:I:1:SER:N	1:I:104:HIS:NE2	2.50	0.60
1:I:134:THR:HB	1:I:140:GLY:HA2	1.82	0.60
1:G:79:TYR:O	1:G:82:THR:HB	2.02	0.60
1:E:37:SER:C	1:E:39:SER:H	2.02	0.60
2:D:67:TYR:N	2:D:67:TYR:CD1	2.69	0.59
1:G:1:SER:N	1:G:104:HIS:NE2	2.50	0.59
1:E:1:SER:N	1:E:104:HIS:NE2	2.50	0.59
1:A:1:SER:N	1:A:104:HIS:NE2	2.50	0.59
1:C:79:TYR:O	1:C:82:THR:HB	2.02	0.59
1:C:1:SER:N	1:C:104:HIS:NE2	2.50	0.59
1:I:79:TYR:O	1:I:82:THR:HB	2.02	0.59
1:E:14:PRO:HG3	1:E:90:ASP:CA	2.26	0.59
1:E:79:TYR:O	1:E:82:THR:HB	2.02	0.59
2:H:67:TYR:N	2:H:67:TYR:CD1	2.69	0.59
2:B:20:SER:CA	2:B:71:THR:HG22	2.28	0.59
2:F:67:TYR:N	2:F:67:TYR:CD1	2.69	0.59
1:G:1:SER:H1	1:G:104:HIS:CE1	2.21	0.59
1:A:79:TYR:O	1:A:82:THR:HB	2.02	0.58
2:H:20:SER:CA	2:H:71:THR:HG22	2.28	0.58
2:H:79:ALA:HB2	2:H:94:LYS:HA	1.86	0.58
1:A:10:VAL:CG1	1:A:77:LEU:HD12	2.33	0.58
1:I:10:VAL:CG1	1:I:77:LEU:HD12	2.33	0.58
1:C:1:SER:H2	1:C:104:HIS:CE1	2.21	0.58
1:I:123:ILE:O	1:I:124:ILE:HG12	2.04	0.58
1:I:14:PRO:HG3	1:I:90:ASP:CA	2.26	0.58
2:J:20:SER:CA	2:J:71:THR:HG22	2.28	0.58
1:C:123:ILE:O	1:C:124:ILE:HG12	2.04	0.58
1:C:10:VAL:CG1	1:C:77:LEU:HD12	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:79:ALA:HB2	2:J:94:LYS:HA	1.86	0.58
1:A:123:ILE:O	1:A:124:ILE:HG12	2.04	0.58
1:G:123:ILE:O	1:G:124:ILE:HG12	2.04	0.58
2:B:79:ALA:HB2	2:B:94:LYS:HA	1.86	0.58
1:A:268:PRO:HD2	1:I:122:TYR:OH	2.04	0.57
1:A:270:THR:HG21	1:I:120:TYR:CE1	2.39	0.57
1:C:253:GLU:O	1:C:255:ARG:N	2.38	0.57
1:A:253:GLU:O	1:A:255:ARG:N	2.38	0.57
1:G:10:VAL:CG1	1:G:77:LEU:HD12	2.33	0.57
1:A:14:PRO:HG3	1:A:90:ASP:CA	2.26	0.57
1:E:253:GLU:O	1:E:255:ARG:N	2.37	0.57
2:F:79:ALA:HB2	2:F:94:LYS:HA	1.86	0.57
1:G:46:PRO:HG3	1:G:59:TRP:CH2	2.40	0.57
1:A:203:TRP:CE3	1:A:243:TRP:HB3	2.40	0.57
1:E:10:VAL:CG1	1:E:77:LEU:HD12	2.33	0.57
1:G:253:GLU:O	1:G:255:ARG:N	2.37	0.57
1:I:203:TRP:CE3	1:I:243:TRP:HB3	2.40	0.57
1:A:1:SER:H2	1:A:104:HIS:CE1	2.23	0.57
1:A:1:SER:N	1:A:104:HIS:CE1	2.73	0.56
1:G:203:TRP:CE3	1:G:243:TRP:HB3	2.40	0.56
1:I:253:GLU:O	1:I:255:ARG:N	2.38	0.56
1:E:1:SER:N	1:E:104:HIS:CE1	2.73	0.56
1:C:46:PRO:HG3	1:C:59:TRP:CZ2	2.40	0.56
1:E:123:ILE:O	1:E:124:ILE:HG12	2.04	0.56
1:I:9:ILE:HD12	1:I:22:ILE:HD11	1.88	0.56
1:I:213:THR:HB	1:I:261:HIS:HB2	1.88	0.56
1:E:203:TRP:CE3	1:E:243:TRP:HB3	2.40	0.56
1:E:46:PRO:HG3	1:E:59:TRP:CZ2	2.40	0.56
1:I:46:PRO:HG3	1:I:59:TRP:CH2	2.40	0.56
1:A:46:PRO:HG3	1:A:59:TRP:CH2	2.40	0.56
1:C:203:TRP:CE3	1:C:243:TRP:HB3	2.40	0.56
1:E:1:SER:H2	1:E:104:HIS:CE1	2.23	0.56
1:G:1:SER:N	1:G:104:HIS:CE1	2.73	0.56
1:I:46:PRO:HG3	1:I:59:TRP:CZ2	2.40	0.56
1:G:199:THR:HA	1:G:246:VAL:O	2.06	0.56
1:I:1:SER:N	1:I:104:HIS:CE1	2.73	0.56
1:A:46:PRO:HG3	1:A:59:TRP:CZ2	2.40	0.56
1:C:199:THR:HA	1:C:246:VAL:O	2.06	0.56
1:G:97:VAL:HG22	2:H:56:PHE:CZ	2.41	0.56
1:A:97:VAL:HG22	2:B:56:PHE:CZ	2.41	0.56
1:C:46:PRO:HG3	1:C:59:TRP:CH2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:199:THR:HA	1:E:246:VAL:O	2.06	0.56
1:C:1:SER:N	1:C:104:HIS:CE1	2.73	0.56
2:D:79:ALA:HB2	2:D:94:LYS:HA	1.86	0.55
1:C:213:THR:HB	1:C:261:HIS:HB2	1.88	0.55
1:E:46:PRO:HG3	1:E:59:TRP:CH2	2.40	0.55
1:E:97:VAL:HG22	2:F:56:PHE:CZ	2.41	0.55
1:C:97:VAL:HG22	2:D:56:PHE:CZ	2.41	0.55
1:G:46:PRO:HG3	1:G:59:TRP:CZ2	2.40	0.55
1:A:213:THR:HB	1:A:261:HIS:HB2	1.88	0.55
1:E:9:ILE:HD12	1:E:22:ILE:HD11	1.88	0.55
1:A:9:ILE:HD12	1:A:22:ILE:HD11	1.88	0.55
1:E:213:THR:HB	1:E:261:HIS:HB2	1.88	0.55
1:G:14:PRO:HG3	1:G:90:ASP:CA	2.26	0.55
1:G:9:ILE:HD12	1:G:22:ILE:HD11	1.88	0.55
1:G:213:THR:HB	1:G:261:HIS:HB2	1.88	0.55
1:C:138:VAL:O	1:C:140:GLY:N	2.39	0.55
1:E:138:VAL:O	1:E:140:GLY:N	2.39	0.55
1:I:97:VAL:HG22	2:J:56:PHE:CZ	2.41	0.55
1:A:199:THR:HA	1:A:246:VAL:O	2.06	0.55
1:I:199:THR:HA	1:I:246:VAL:O	2.06	0.55
1:C:9:ILE:HD12	1:C:22:ILE:HD11	1.88	0.54
3:G:304:NAG:H3	3:G:304:NAG:H83	1.90	0.54
1:G:10:VAL:HG21	1:G:73:ALA:HB1	1.89	0.54
1:C:10:VAL:HG21	1:C:73:ALA:HB1	1.89	0.54
1:A:10:VAL:HG21	1:A:73:ALA:HB1	1.89	0.54
1:G:212:ILE:HG12	1:G:213:THR:N	2.23	0.54
1:A:138:VAL:O	1:A:140:GLY:N	2.39	0.54
1:I:212:ILE:HG12	1:I:213:THR:N	2.23	0.54
1:I:138:VAL:O	1:I:140:GLY:N	2.39	0.54
1:C:212:ILE:HG12	1:C:213:THR:N	2.23	0.54
1:G:271:LEU:N	1:G:271:LEU:HD12	2.23	0.54
3:I:305:NAG:H83	3:I:305:NAG:H3	1.90	0.54
1:C:271:LEU:N	1:C:271:LEU:HD12	2.23	0.53
3:E:303:NAG:H3	3:E:303:NAG:H83	1.90	0.53
1:G:138:VAL:O	1:G:140:GLY:N	2.39	0.53
1:I:1:SER:H2	1:I:104:HIS:CE1	2.26	0.53
1:E:10:VAL:HG21	1:E:73:ALA:HB1	1.89	0.53
1:E:212:ILE:HG12	1:E:213:THR:N	2.23	0.53
3:C:302:NAG:H83	3:C:302:NAG:H3	1.90	0.53
1:A:271:LEU:N	1:A:271:LEU:HD12	2.23	0.53
1:I:10:VAL:HG21	1:I:73:ALA:HB1	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:ILE:HG12	1:A:213:THR:N	2.23	0.53
1:I:271:LEU:HD12	1:I:271:LEU:N	2.23	0.53
1:G:270:THR:C	1:G:271:LEU:HD12	2.30	0.52
3:A:301:NAG:H83	3:A:301:NAG:H3	1.90	0.52
1:E:271:LEU:N	1:E:271:LEU:HD12	2.23	0.52
1:G:76:THR:O	1:G:80:MET:HG3	2.10	0.52
1:A:270:THR:C	1:A:271:LEU:HD12	2.30	0.52
1:C:270:THR:C	1:C:271:LEU:HD12	2.30	0.52
1:E:270:THR:C	1:E:271:LEU:HD12	2.30	0.52
1:E:76:THR:O	1:E:80:MET:HG3	2.10	0.52
2:H:51:HIS:HA	2:H:65:LEU:O	2.09	0.52
1:I:270:THR:C	1:I:271:LEU:HD12	2.30	0.52
2:J:49:VAL:HA	2:J:68:THR:HG23	1.92	0.52
2:B:51:HIS:HA	2:B:65:LEU:O	2.10	0.52
1:A:76:THR:O	1:A:80:MET:HG3	2.10	0.52
2:B:49:VAL:HA	2:B:68:THR:HG23	1.92	0.52
1:C:76:THR:O	1:C:80:MET:HG3	2.10	0.52
1:C:12:MET:HB2	1:C:92:HIS:HB2	1.92	0.52
2:D:51:HIS:HA	2:D:65:LEU:O	2.09	0.52
1:I:12:MET:HB2	1:I:92:HIS:HB2	1.92	0.52
1:G:116:THR:HG23	1:G:122:TYR:CD2	2.45	0.51
1:A:12:MET:HB2	1:A:92:HIS:HB2	1.92	0.51
2:F:51:HIS:HA	2:F:65:LEU:O	2.09	0.51
1:G:27:VAL:HG11	1:G:178:LEU:HD11	1.93	0.51
1:I:116:THR:HG23	1:I:122:TYR:CD2	2.45	0.51
1:A:116:THR:HG23	1:A:122:TYR:CD2	2.45	0.51
1:E:3:TRP:CZ2	1:E:101:ASN:HB2	2.46	0.51
1:E:116:THR:HG23	1:E:122:TYR:CD2	2.45	0.51
1:I:76:THR:O	1:I:80:MET:HG3	2.10	0.51
2:B:79:ALA:CB	2:B:94:LYS:HA	2.40	0.51
1:G:3:TRP:CZ2	1:G:101:ASN:HB2	2.46	0.51
2:H:79:ALA:CB	2:H:94:LYS:HA	2.40	0.51
1:I:27:VAL:HG11	1:I:178:LEU:HD11	1.93	0.51
1:A:270:THR:CG2	1:I:120:TYR:CE1	2.94	0.51
1:A:3:TRP:CZ2	1:A:101:ASN:HB2	2.46	0.51
1:C:116:THR:HG23	1:C:122:TYR:CD2	2.45	0.51
1:A:27:VAL:HG11	1:A:178:LEU:HD11	1.93	0.51
1:E:27:VAL:HG11	1:E:178:LEU:HD11	1.93	0.51
2:D:79:ALA:CB	2:D:94:LYS:HA	2.40	0.51
2:H:49:VAL:HA	2:H:68:THR:HG23	1.92	0.51
1:I:3:TRP:CZ2	1:I:101:ASN:HB2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:51:HIS:HA	2:J:65:LEU:O	2.09	0.51
2:J:79:ALA:CB	2:J:94:LYS:HA	2.40	0.51
1:I:138:VAL:C	1:I:140:GLY:H	2.14	0.50
2:F:49:VAL:HA	2:F:68:THR:HG23	1.92	0.50
2:F:79:ALA:CB	2:F:94:LYS:HA	2.40	0.50
1:G:12:MET:HB2	1:G:92:HIS:HB2	1.92	0.50
1:C:116:THR:HG22	1:C:117:TYR:N	2.27	0.50
1:C:138:VAL:C	1:C:140:GLY:H	2.14	0.50
1:I:116:THR:HG22	1:I:117:TYR:N	2.27	0.50
1:A:270:THR:HB	1:I:120:TYR:CE1	2.46	0.50
2:D:49:VAL:HA	2:D:68:THR:HG23	1.92	0.50
1:C:3:TRP:CZ2	1:C:101:ASN:HB2	2.45	0.50
1:E:116:THR:HG22	1:E:117:TYR:N	2.27	0.50
1:A:9:ILE:HD12	1:A:22:ILE:CD1	2.42	0.50
1:E:138:VAL:C	1:E:140:GLY:H	2.14	0.50
1:C:27:VAL:HG11	1:C:178:LEU:HD11	1.93	0.49
1:E:12:MET:HB2	1:E:92:HIS:HB2	1.92	0.49
1:G:138:VAL:C	1:G:140:GLY:H	2.14	0.49
1:A:116:THR:HG22	1:A:117:TYR:N	2.27	0.49
1:E:227:MET:CB	1:E:246:VAL:HG12	2.42	0.49
1:G:116:THR:HG22	1:G:117:TYR:N	2.27	0.49
1:G:227:MET:CB	1:G:246:VAL:HG12	2.43	0.49
1:G:9:ILE:HD12	1:G:22:ILE:CD1	2.42	0.49
1:I:227:MET:CB	1:I:246:VAL:HG12	2.42	0.49
1:A:227:MET:CB	1:A:246:VAL:HG12	2.43	0.49
1:I:219:ASP:N	1:I:255:ARG:O	2.40	0.49
1:G:44:MET:HG2	1:G:62:GLU:HB3	1.95	0.49
1:A:44:MET:HG2	1:A:62:GLU:HB3	1.95	0.49
1:G:199:THR:CG2	1:G:247:VAL:HG12	2.42	0.49
1:A:138:VAL:C	1:A:140:GLY:H	2.14	0.49
1:A:228:GLU:HG2	1:A:230:PRO:HD3	1.95	0.49
1:C:227:MET:CB	1:C:246:VAL:HG12	2.42	0.49
1:E:9:ILE:HD12	1:E:22:ILE:CD1	2.42	0.49
1:I:199:THR:CG2	1:I:247:VAL:HG12	2.42	0.49
1:C:9:ILE:HD12	1:C:22:ILE:CD1	2.42	0.48
1:G:127:GLU:C	1:G:129:LEU:H	2.17	0.48
2:B:76:ASP:HB3	2:B:78:TYR:CE1	2.48	0.48
1:E:44:MET:HG2	1:E:62:GLU:HB3	1.95	0.48
1:I:44:MET:HG2	1:I:62:GLU:HB3	1.95	0.48
1:A:189:THR:OG1	1:A:201:ARG:HB3	2.13	0.48
1:C:44:MET:HG2	1:C:62:GLU:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:199:THR:CG2	1:E:247:VAL:HG12	2.42	0.48
1:G:189:THR:OG1	1:G:201:ARG:HB3	2.13	0.48
1:I:9:ILE:HD12	1:I:22:ILE:CD1	2.42	0.48
2:F:76:ASP:HB3	2:F:78:TYR:CE1	2.49	0.48
1:G:228:GLU:HG2	1:G:230:PRO:HD3	1.95	0.48
1:A:35:PHE:C	1:A:35:PHE:CD1	2.87	0.48
2:D:76:ASP:HB3	2:D:78:TYR:CE1	2.48	0.48
1:E:228:GLU:HG2	1:E:230:PRO:HD3	1.95	0.48
1:E:189:THR:OG1	1:E:201:ARG:HB3	2.13	0.48
1:E:55:PRO:O	1:E:58:TYR:HB3	2.14	0.48
1:A:199:THR:CG2	1:A:247:VAL:HG12	2.42	0.48
1:A:55:PRO:O	1:A:58:TYR:HB3	2.14	0.48
1:C:125:LEU:HD13	1:C:132:TRP:CZ2	2.49	0.48
1:E:127:GLU:C	1:E:129:LEU:H	2.17	0.48
1:E:125:LEU:HD13	1:E:132:TRP:CZ2	2.49	0.48
1:G:55:PRO:O	1:G:58:TYR:HB3	2.14	0.48
1:A:270:THR:HG21	1:I:120:TYR:HE1	1.79	0.48
1:C:35:PHE:CD1	1:C:35:PHE:C	2.87	0.48
1:I:189:THR:OG1	1:I:201:ARG:HB3	2.13	0.48
1:A:77:LEU:HG	1:A:94:LEU:HB2	1.96	0.47
1:C:228:GLU:HG2	1:C:230:PRO:HD3	1.95	0.47
1:C:219:ASP:N	1:C:255:ARG:O	2.40	0.47
1:G:125:LEU:HD13	1:G:132:TRP:CZ2	2.49	0.47
1:G:77:LEU:HG	1:G:94:LEU:HB2	1.96	0.47
2:H:76:ASP:HB3	2:H:78:TYR:CE1	2.48	0.47
2:J:76:ASP:HB3	2:J:78:TYR:CE1	2.49	0.47
1:C:189:THR:OG1	1:C:201:ARG:HB3	2.13	0.47
1:E:35:PHE:C	1:E:35:PHE:CD1	2.87	0.47
1:G:219:ASP:N	1:G:255:ARG:O	2.40	0.47
1:I:10:VAL:CG2	1:I:73:ALA:HB1	2.44	0.47
1:A:113:TYR:CD2	1:A:113:TYR:C	2.88	0.47
1:A:125:LEU:HD13	1:A:132:TRP:CZ2	2.49	0.47
1:C:10:VAL:CG2	1:C:73:ALA:HB1	2.44	0.47
1:G:10:VAL:CG2	1:G:73:ALA:HB1	2.44	0.47
1:A:10:VAL:CG2	1:A:73:ALA:HB1	2.44	0.47
1:C:199:THR:CG2	1:C:247:VAL:HG12	2.42	0.47
1:C:55:PRO:O	1:C:58:TYR:HB3	2.14	0.47
1:I:127:GLU:C	1:I:129:LEU:H	2.17	0.47
1:E:113:TYR:CD2	1:E:113:TYR:C	2.88	0.47
1:G:35:PHE:CD1	1:G:35:PHE:C	2.87	0.47
1:A:198:VAL:N	1:A:248:VAL:O	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:198:VAL:O	1:C:247:VAL:HA	2.15	0.47
1:E:198:VAL:O	1:E:247:VAL:HA	2.15	0.47
1:I:198:VAL:N	1:I:248:VAL:O	2.48	0.47
1:E:77:LEU:HG	1:E:94:LEU:HB2	1.96	0.47
1:I:113:TYR:CD2	1:I:113:TYR:C	2.88	0.47
1:I:55:PRO:O	1:I:58:TYR:HB3	2.14	0.47
1:C:127:GLU:C	1:C:129:LEU:H	2.17	0.47
1:G:198:VAL:N	1:G:248:VAL:O	2.48	0.47
1:I:125:LEU:HD13	1:I:132:TRP:CZ2	2.49	0.47
1:A:212:ILE:HG12	1:A:213:THR:H	1.80	0.47
1:I:228:GLU:HG2	1:I:230:PRO:HD3	1.95	0.47
1:I:35:PHE:CD1	1:I:35:PHE:C	2.87	0.47
1:A:127:GLU:C	1:A:129:LEU:H	2.17	0.47
1:E:198:VAL:N	1:E:248:VAL:O	2.48	0.47
1:E:212:ILE:HG12	1:E:213:THR:H	1.80	0.47
1:G:198:VAL:O	1:G:247:VAL:HA	2.15	0.47
1:C:198:VAL:N	1:C:248:VAL:O	2.48	0.47
1:C:212:ILE:HG12	1:C:213:THR:H	1.80	0.46
1:E:10:VAL:CG2	1:E:73:ALA:HB1	2.44	0.46
1:C:77:LEU:HG	1:C:94:LEU:HB2	1.96	0.46
1:G:116:THR:CG2	1:G:122:TYR:CE2	2.98	0.46
1:G:212:ILE:HG12	1:G:213:THR:H	1.80	0.46
1:I:116:THR:CG2	1:I:122:TYR:CE2	2.98	0.46
1:I:269:LEU:HA	1:I:269:LEU:HD12	1.70	0.46
1:I:77:LEU:HG	1:I:94:LEU:HB2	1.96	0.46
1:G:113:TYR:C	1:G:113:TYR:CD2	2.88	0.46
1:I:198:VAL:O	1:I:247:VAL:HA	2.15	0.46
1:A:198:VAL:O	1:A:247:VAL:HA	2.15	0.46
1:E:219:ASP:N	1:E:255:ARG:O	2.40	0.46
1:I:27:VAL:CG1	1:I:27:VAL:O	2.63	0.46
1:C:113:TYR:CD2	1:C:113:TYR:C	2.88	0.46
1:G:27:VAL:O	1:G:27:VAL:CG1	2.63	0.46
1:C:27:VAL:CG1	1:C:27:VAL:O	2.63	0.46
1:E:116:THR:CG2	1:E:122:TYR:CE2	2.98	0.46
1:G:183:ALA:HB2	1:G:264:GLY:O	2.16	0.46
1:A:116:THR:CG2	1:A:122:TYR:CE2	2.98	0.46
1:A:266:PRO:HB2	1:I:122:TYR:CG	2.51	0.46
1:A:27:VAL:O	1:A:27:VAL:CG1	2.63	0.46
1:I:32:TYR:CD2	1:I:33:GLN:HG3	2.51	0.46
1:I:183:ALA:HB2	1:I:264:GLY:O	2.16	0.46
1:C:116:THR:CG2	1:C:122:TYR:CE2	2.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:32:TYR:CD2	1:C:33:GLN:HG3	2.51	0.45
1:E:27:VAL:O	1:E:27:VAL:CG1	2.63	0.45
1:I:273:TRP:CE3	1:I:274:GLY:N	2.85	0.45
1:E:273:TRP:CE3	1:E:274:GLY:N	2.84	0.45
1:E:32:TYR:CD2	1:E:33:GLN:HG3	2.51	0.45
2:H:25:CYS:HB2	2:H:39:LEU:HD21	1.98	0.45
1:A:183:ALA:HB2	1:A:264:GLY:O	2.16	0.45
1:A:273:TRP:CE3	1:A:274:GLY:N	2.85	0.45
1:A:32:TYR:CD2	1:A:33:GLN:HG3	2.51	0.45
2:B:25:CYS:HB2	2:B:39:LEU:HD21	1.98	0.45
1:C:183:ALA:HB2	1:C:264:GLY:O	2.16	0.45
1:C:97:VAL:HG22	2:D:56:PHE:HZ	1.81	0.45
1:I:97:VAL:HG22	2:J:56:PHE:HZ	1.81	0.45
2:J:25:CYS:HB2	2:J:39:LEU:HD21	1.98	0.45
1:A:10:VAL:HB	1:A:94:LEU:HB3	1.99	0.45
1:C:10:VAL:HB	1:C:94:LEU:HB3	1.99	0.45
1:E:118:TYR:CD2	2:F:31:HIS:CE1	3.05	0.45
1:G:118:TYR:CD2	2:H:31:HIS:CE1	3.05	0.45
1:I:37:SER:C	1:I:39:SER:N	2.70	0.45
1:I:10:VAL:HB	1:I:94:LEU:HB3	1.98	0.45
1:A:210:ALA:HB2	1:A:240:PHE:CE1	2.52	0.45
1:A:37:SER:C	1:A:39:SER:N	2.70	0.45
2:D:25:CYS:HB2	2:D:39:LEU:HD21	1.98	0.45
1:E:210:ALA:HB2	1:E:240:PHE:CE1	2.52	0.45
1:G:210:ALA:HB2	1:G:240:PHE:CE1	2.52	0.45
1:G:32:TYR:CD2	1:G:33:GLN:HG3	2.51	0.45
1:I:118:TYR:CD2	2:J:31:HIS:CE1	3.05	0.45
1:A:118:TYR:CD2	2:B:31:HIS:CE1	3.05	0.45
1:E:37:SER:C	1:E:39:SER:N	2.70	0.45
1:C:273:TRP:CE3	1:C:274:GLY:N	2.85	0.45
1:C:118:TYR:CD2	2:D:31:HIS:CE1	3.05	0.45
1:I:157:THR:O	1:I:158:TYR:C	2.54	0.45
1:G:273:TRP:CE3	1:G:274:GLY:N	2.85	0.45
1:E:127:GLU:C	1:E:129:LEU:N	2.71	0.45
1:C:37:SER:C	1:C:39:SER:N	2.70	0.44
1:E:10:VAL:HB	1:E:94:LEU:HB3	1.98	0.44
1:I:127:GLU:C	1:I:129:LEU:N	2.71	0.44
1:A:97:VAL:HG22	2:B:56:PHE:HZ	1.81	0.44
1:C:157:THR:O	1:C:158:TYR:C	2.54	0.44
1:C:210:ALA:HB2	1:C:240:PHE:CE1	2.52	0.44
1:G:10:VAL:HB	1:G:94:LEU:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:157:THR:O	1:E:158:TYR:C	2.54	0.44
1:E:183:ALA:HB2	1:E:264:GLY:O	2.16	0.44
1:E:251:GLY:C	1:E:253:GLU:H	2.21	0.44
1:E:97:VAL:HG22	2:F:56:PHE:HZ	1.81	0.44
1:G:127:GLU:C	1:G:129:LEU:N	2.71	0.44
1:I:218:ARG:HA	1:I:255:ARG:O	2.18	0.44
2:B:20:SER:O	2:B:21:ASN:HB2	2.18	0.44
1:A:157:THR:O	1:A:158:TYR:C	2.54	0.44
1:A:230:PRO:HG2	1:A:243:TRP:CZ2	2.53	0.44
1:C:230:PRO:HG2	1:C:243:TRP:CZ2	2.53	0.44
1:E:138:VAL:HG12	1:E:139:GLY:N	2.33	0.44
1:G:97:VAL:HG22	2:H:56:PHE:HZ	1.81	0.44
1:I:212:ILE:HG12	1:I:213:THR:H	1.80	0.44
1:I:210:ALA:HB2	1:I:240:PHE:CE1	2.52	0.44
1:A:218:ARG:HA	1:A:255:ARG:O	2.18	0.44
1:G:138:VAL:HG12	1:G:139:GLY:N	2.33	0.44
1:I:138:VAL:HG12	1:I:139:GLY:N	2.33	0.44
2:J:23:LEU:O	2:J:67:TYR:HA	2.18	0.44
1:C:251:GLY:C	1:C:253:GLU:H	2.21	0.43
2:D:20:SER:O	2:D:21:ASN:HB2	2.18	0.43
1:G:157:THR:O	1:G:158:TYR:C	2.54	0.43
1:E:218:ARG:HA	1:E:255:ARG:O	2.18	0.43
2:F:20:SER:O	2:F:21:ASN:HB2	2.18	0.43
2:F:25:CYS:HB2	2:F:39:LEU:HD21	1.98	0.43
1:G:218:ARG:HA	1:G:255:ARG:O	2.18	0.43
1:A:251:GLY:C	1:A:253:GLU:H	2.21	0.43
2:D:23:LEU:O	2:D:67:TYR:HA	2.18	0.43
2:F:23:LEU:O	2:F:67:TYR:HA	2.18	0.43
1:C:127:GLU:C	1:C:129:LEU:N	2.71	0.43
1:A:127:GLU:C	1:A:129:LEU:N	2.71	0.43
1:A:77:LEU:HD21	1:A:92:HIS:HB3	2.01	0.43
1:C:138:VAL:HG12	1:C:139:GLY:N	2.33	0.43
1:C:134:THR:CB	1:C:139:GLY:O	2.66	0.43
1:I:77:LEU:HD21	1:I:92:HIS:HB3	2.01	0.43
1:A:138:VAL:HG12	1:A:139:GLY:N	2.33	0.43
2:D:48:LYS:O	2:D:68:THR:CG2	2.67	0.43
1:E:230:PRO:HG2	1:E:243:TRP:CZ2	2.53	0.43
2:F:48:LYS:O	2:F:68:THR:CG2	2.67	0.43
1:G:116:THR:HG23	1:G:122:TYR:CE2	2.54	0.43
1:G:37:SER:C	1:G:39:SER:N	2.70	0.43
2:H:20:SER:O	2:H:21:ASN:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:116:THR:HG23	1:I:122:TYR:CE2	2.54	0.43
1:G:188:VAL:HG12	1:G:189:THR:N	2.34	0.43
1:I:230:PRO:HG2	1:I:243:TRP:CZ2	2.53	0.43
1:C:116:THR:HG23	1:C:122:TYR:CE2	2.54	0.42
1:C:218:ARG:HA	1:C:255:ARG:O	2.18	0.42
1:E:77:LEU:HD21	1:E:92:HIS:HB3	2.01	0.42
1:G:199:THR:HG22	1:G:247:VAL:CG1	2.48	0.42
2:B:23:LEU:O	2:B:67:TYR:HA	2.18	0.42
2:B:48:LYS:O	2:B:68:THR:CG2	2.67	0.42
1:C:106:GLY:HA2	1:C:168:LEU:HD21	2.01	0.42
1:E:116:THR:HG23	1:E:122:TYR:CE2	2.54	0.42
1:G:77:LEU:HD21	1:G:92:HIS:HB3	2.01	0.42
2:H:23:LEU:O	2:H:67:TYR:HA	2.18	0.42
2:J:48:LYS:O	2:J:68:THR:CG2	2.67	0.42
1:G:106:GLY:HA2	1:G:168:LEU:HD21	2.01	0.42
1:G:251:GLY:C	1:G:253:GLU:H	2.21	0.42
2:H:48:LYS:O	2:H:68:THR:CG2	2.67	0.42
1:I:106:GLY:HA2	1:I:168:LEU:HD21	2.01	0.42
1:I:251:GLY:C	1:I:253:GLU:H	2.21	0.42
2:J:20:SER:O	2:J:21:ASN:HB2	2.18	0.42
1:A:80:MET:HE2	1:A:138:VAL:HB	2.02	0.42
1:A:212:ILE:HG13	1:A:262:HIS:HB2	2.02	0.42
1:G:230:PRO:HG2	1:G:243:TRP:CZ2	2.53	0.42
1:A:266:PRO:HB2	1:I:122:TYR:CD2	2.54	0.42
2:B:17:ASN:C	2:B:19:LYS:H	2.23	0.42
1:C:185:ARG:HG3	1:C:185:ARG:HH11	1.85	0.42
1:G:185:ARG:HG3	1:G:185:ARG:HH11	1.85	0.42
1:C:80:MET:HE2	1:C:138:VAL:HB	2.02	0.42
1:E:106:GLY:HA2	1:E:168:LEU:HD21	2.01	0.42
1:E:214:LEU:CD2	1:E:260:VAL:HG22	2.50	0.42
1:I:214:LEU:CD2	1:I:260:VAL:HG22	2.50	0.42
1:A:214:LEU:CD2	1:A:260:VAL:HG22	2.50	0.42
1:C:128:ASP:C	1:C:130:ASN:N	2.73	0.42
2:D:17:ASN:C	2:D:19:LYS:H	2.23	0.42
1:E:188:VAL:HG12	1:E:189:THR:N	2.34	0.42
2:F:17:ASN:C	2:F:19:LYS:H	2.23	0.42
2:F:37:VAL:HG11	2:F:66:TYR:CD1	2.55	0.42
1:G:54:GLU:HA	1:G:55:PRO:HD3	1.84	0.42
2:J:37:VAL:HG11	2:J:66:TYR:CD1	2.55	0.42
1:A:134:THR:CB	1:A:139:GLY:O	2.66	0.42
2:B:37:VAL:HG11	2:B:66:TYR:CD1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:273:TRP:HA	1:C:273:TRP:CE3	2.55	0.42
2:D:37:VAL:HG11	2:D:66:TYR:CD1	2.55	0.42
1:E:185:ARG:HG3	1:E:185:ARG:HH11	1.85	0.42
1:I:188:VAL:HG12	1:I:189:THR:N	2.34	0.42
1:I:51:MET:C	1:I:53:GLN:H	2.22	0.42
1:A:51:MET:C	1:A:53:GLN:H	2.22	0.42
1:C:212:ILE:HG13	1:C:262:HIS:HB2	2.02	0.42
1:E:134:THR:CB	1:E:139:GLY:O	2.66	0.42
1:E:273:TRP:HA	1:E:273:TRP:CE3	2.55	0.42
1:G:80:MET:HE2	1:G:138:VAL:HB	2.02	0.42
1:G:51:MET:C	1:G:53:GLN:H	2.22	0.42
1:A:116:THR:HG23	1:A:122:TYR:CE2	2.54	0.42
1:A:19:PRO:O	1:A:74:ARG:NH1	2.53	0.42
1:E:128:ASP:O	1:E:130:ASN:N	2.53	0.42
1:E:212:ILE:HG13	1:E:262:HIS:HB2	2.02	0.42
1:G:123:ILE:HG22	1:G:123:ILE:O	2.20	0.42
1:I:273:TRP:HE3	1:I:273:TRP:HA	1.85	0.42
1:A:249:PRO:O	1:A:250:PHE:C	2.59	0.41
1:C:128:ASP:O	1:C:130:ASN:N	2.53	0.41
1:C:77:LEU:HD21	1:C:92:HIS:HB3	2.01	0.41
1:G:128:ASP:C	1:G:130:ASN:N	2.73	0.41
1:G:214:LEU:CD2	1:G:260:VAL:HG22	2.50	0.41
1:I:249:PRO:O	1:I:250:PHE:C	2.59	0.41
1:A:128:ASP:O	1:A:130:ASN:N	2.53	0.41
1:E:249:PRO:O	1:E:250:PHE:C	2.59	0.41
1:E:51:MET:C	1:E:53:GLN:H	2.22	0.41
1:A:273:TRP:CE3	1:A:273:TRP:HA	2.55	0.41
1:A:273:TRP:HE3	1:A:273:TRP:HA	1.85	0.41
1:A:97:VAL:HG22	2:B:56:PHE:CE1	2.55	0.41
1:C:19:PRO:O	1:C:74:ARG:NH1	2.53	0.41
1:C:214:LEU:CD2	1:C:260:VAL:HG22	2.50	0.41
1:E:97:VAL:HG22	2:F:56:PHE:CE1	2.55	0.41
1:I:128:ASP:O	1:I:130:ASN:N	2.53	0.41
1:A:128:ASP:C	1:A:130:ASN:N	2.73	0.41
1:E:199:THR:HG22	1:E:247:VAL:CG1	2.48	0.41
2:H:37:VAL:HG11	2:H:66:TYR:CD1	2.55	0.41
1:I:80:MET:HE2	1:I:138:VAL:HB	2.02	0.41
1:I:19:PRO:O	1:I:74:ARG:NH1	2.53	0.41
2:J:17:ASN:C	2:J:19:LYS:H	2.23	0.41
1:A:199:THR:HG22	1:A:247:VAL:CG1	2.48	0.41
1:C:188:VAL:HG12	1:C:189:THR:N	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:84:HIS:CE1	2:D:86:THR:HG23	2.56	0.41
2:H:17:ASN:C	2:H:19:LYS:H	2.23	0.41
1:I:128:ASP:C	1:I:130:ASN:N	2.73	0.41
1:I:97:VAL:HG22	2:J:56:PHE:CE1	2.55	0.41
1:A:185:ARG:HH11	1:A:185:ARG:HG3	1.85	0.41
3:A:301:NAG:C7	3:A:301:NAG:O3	2.68	0.41
1:C:249:PRO:O	1:C:250:PHE:C	2.59	0.41
1:C:51:MET:C	1:C:53:GLN:H	2.22	0.41
1:E:269:LEU:HA	1:E:269:LEU:HD12	1.70	0.41
1:I:123:ILE:HG22	1:I:123:ILE:O	2.20	0.41
1:I:273:TRP:HA	1:I:273:TRP:CE3	2.55	0.41
1:A:123:ILE:HG22	1:A:123:ILE:O	2.20	0.41
1:C:273:TRP:HA	1:C:273:TRP:HE3	1.85	0.41
1:G:128:ASP:O	1:G:130:ASN:N	2.53	0.41
1:G:249:PRO:O	1:G:250:PHE:C	2.59	0.41
1:G:273:TRP:HA	1:G:273:TRP:HE3	1.85	0.41
1:I:1:SER:H2	1:I:104:HIS:CD2	2.38	0.41
1:C:168:LEU:HD23	1:C:168:LEU:HA	1.89	0.41
1:E:19:PRO:O	1:E:74:ARG:NH1	2.53	0.41
1:E:273:TRP:HE3	1:E:273:TRP:HA	1.85	0.41
1:G:19:PRO:O	1:G:74:ARG:NH1	2.53	0.41
1:G:273:TRP:HA	1:G:273:TRP:CE3	2.55	0.41
1:I:183:ALA:HA	1:I:184:PRO:HD3	1.89	0.41
1:I:199:THR:HG22	1:I:247:VAL:CG1	2.48	0.41
1:I:212:ILE:HG13	1:I:262:HIS:HB2	2.02	0.41
2:B:24:ASN:HB3	2:B:65:LEU:HD11	2.03	0.41
2:B:24:ASN:OD1	2:B:67:TYR:HB3	2.21	0.41
2:D:24:ASN:OD1	2:D:67:TYR:HB3	2.21	0.41
1:E:80:MET:HE2	1:E:138:VAL:HB	2.02	0.41
2:F:84:HIS:CE1	2:F:86:THR:HG23	2.56	0.41
1:I:77:LEU:CD2	1:I:81:VAL:HG23	2.51	0.41
1:A:188:VAL:HG12	1:A:189:THR:N	2.34	0.41
1:C:97:VAL:HG22	2:D:56:PHE:CE1	2.55	0.41
2:D:51:HIS:HB3	2:D:66:TYR:CD2	2.56	0.41
1:E:123:ILE:O	1:E:123:ILE:HG22	2.20	0.41
2:F:38:ASP:O	2:F:80:CYS:HA	2.21	0.41
1:G:97:VAL:HG22	2:H:56:PHE:CE1	2.55	0.41
1:I:133:THR:O	1:I:133:THR:HG22	2.21	0.41
2:J:24:ASN:HB3	2:J:65:LEU:HD11	2.03	0.41
1:E:217:LYS:O	1:E:256:TYR:HA	2.22	0.41
1:G:212:ILE:HG13	1:G:262:HIS:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:116:THR:HG21	1:I:122:TYR:CE2	2.56	0.41
2:J:24:ASN:OD1	2:J:67:TYR:HB3	2.21	0.41
1:A:266:PRO:HB3	1:I:124:ILE:HD12	2.02	0.40
1:A:82:THR:O	1:A:85:ASN:N	2.44	0.40
2:F:51:HIS:HB3	2:F:66:TYR:CD2	2.56	0.40
1:G:269:LEU:HD12	1:G:269:LEU:HA	1.70	0.40
2:H:84:HIS:CE1	2:H:86:THR:HG23	2.56	0.40
2:J:51:HIS:HB3	2:J:66:TYR:CD2	2.56	0.40
1:A:217:LYS:O	1:A:256:TYR:HA	2.22	0.40
2:B:84:HIS:CE1	2:B:86:THR:HG23	2.56	0.40
1:E:116:THR:HG21	1:E:122:TYR:CE2	2.56	0.40
1:A:45:GLN:HA	1:A:46:PRO:HD3	1.90	0.40
1:C:123:ILE:O	1:C:123:ILE:HG22	2.20	0.40
1:C:217:LYS:O	1:C:256:TYR:HA	2.22	0.40
2:D:38:ASP:O	2:D:80:CYS:HA	2.21	0.40
1:E:138:VAL:C	1:E:140:GLY:N	2.75	0.40
1:G:133:THR:HG22	1:G:133:THR:O	2.21	0.40
1:I:138:VAL:C	1:I:140:GLY:N	2.75	0.40
1:A:106:GLY:HA2	1:A:168:LEU:HD21	2.01	0.40
1:C:138:VAL:C	1:C:140:GLY:N	2.75	0.40
2:F:24:ASN:OD1	2:F:67:TYR:HB3	2.21	0.40
1:G:225:GLN:C	1:G:227:MET:H	2.25	0.40
2:H:24:ASN:OD1	2:H:67:TYR:HB3	2.21	0.40
2:B:51:HIS:HB3	2:B:66:TYR:CD2	2.56	0.40
1:C:116:THR:HG21	1:C:122:TYR:CE2	2.56	0.40
1:C:77:LEU:CD2	1:C:81:VAL:HG23	2.51	0.40
1:G:116:THR:HG21	1:G:122:TYR:CE2	2.56	0.40
2:H:51:HIS:HB3	2:H:66:TYR:CD2	2.56	0.40
2:J:38:ASP:O	2:J:80:CYS:HA	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:C:268:PRO:CD	1:E:122:TYR:OH[2_565]	2.08	0.12

## 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	253/274 (92%)	213 (84%)	32 (13%)	8 (3%)	4	22
1	C	253/274 (92%)	213 (84%)	32 (13%)	8 (3%)	4	22
1	E	253/274 (92%)	213 (84%)	32 (13%)	8 (3%)	4	22
1	G	253/274 (92%)	213 (84%)	32 (13%)	8 (3%)	4	22
1	I	253/274 (92%)	213 (84%)	32 (13%)	8 (3%)	4	22
2	B	97/99 (98%)	84 (87%)	9 (9%)	4 (4%)	3	16
2	D	97/99 (98%)	84 (87%)	9 (9%)	4 (4%)	3	16
2	F	97/99 (98%)	84 (87%)	8 (8%)	5 (5%)	2	12
2	H	97/99 (98%)	84 (87%)	8 (8%)	5 (5%)	2	12
2	J	97/99 (98%)	84 (87%)	9 (9%)	4 (4%)	3	16
All	All	1750/1865 (94%)	1485 (85%)	203 (12%)	62 (4%)	3	20

All (62) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	90	ASP
1	A	226	ASP
1	A	230	PRO
1	A	254	LEU
2	B	47	GLU
1	C	90	ASP
1	C	226	ASP
1	C	230	PRO
1	C	254	LEU
2	D	47	GLU
1	E	90	ASP
1	E	226	ASP
1	E	230	PRO
1	E	254	LEU

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Mol	Chain	Res	Type
2	F	47	GLU
1	G	90	ASP
1	G	226	ASP
1	G	230	PRO
1	G	254	LEU
2	H	47	GLU
1	I	90	ASP
1	I	226	ASP
1	I	230	PRO
1	I	254	LEU
2	J	47	GLU
1	A	129	LEU
1	C	129	LEU
1	E	129	LEU
1	G	129	LEU
1	I	129	LEU
1	A	87	LYS
1	A	263	GLU
2	B	21	ASN
1	C	87	LYS
1	C	263	GLU
2	D	21	ASN
1	E	87	LYS
1	E	263	GLU
2	F	21	ASN
1	G	87	LYS
1	G	263	GLU
2	H	21	ASN
1	I	87	LYS
1	I	263	GLU
2	J	21	ASN
2	B	20	SER
2	B	48	LYS
2	D	20	SER
2	D	48	LYS
2	F	20	SER
2	F	48	LYS
2	H	20	SER
2	H	48	LYS
2	J	20	SER
2	J	48	LYS
2	F	15	ALA

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Mol	Chain	Res	Type
2	H	15	ALA
1	A	139	GLY
1	C	139	GLY
1	E	139	GLY
1	G	139	GLY
1	I	139	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	A	185/235 (79%)	172 (93%)	13 (7%)	15	47
1	C	185/235 (79%)	172 (93%)	13 (7%)	15	47
1	E	185/235 (79%)	172 (93%)	13 (7%)	15	47
1	G	185/235 (79%)	172 (93%)	13 (7%)	15	47
1	I	185/235 (79%)	172 (93%)	13 (7%)	15	47
2	B	79/94 (84%)	75 (95%)	4 (5%)	24	60
2	D	79/94 (84%)	75 (95%)	4 (5%)	24	60
2	F	79/94 (84%)	75 (95%)	4 (5%)	24	60
2	H	79/94 (84%)	75 (95%)	4 (5%)	24	60
2	J	79/94 (84%)	75 (95%)	4 (5%)	24	60
All	All	1320/1645 (80%)	1235 (94%)	85 (6%)	17	51

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	ILE
1	A	45	GLN
1	A	72	LEU
1	A	77	LEU
1	A	90	ASP
1	A	97	VAL
1	A	101	ASN

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Mol	Chain	Res	Type
1	A	116	THR
1	A	117	TYR
1	A	123	ILE
1	A	124	ILE
1	A	170	CYS
1	A	273	TRP
2	B	67	TYR
2	B	68	THR
2	B	70	PHE
2	B	90	PRO
1	C	22	ILE
1	C	45	GLN
1	C	72	LEU
1	C	77	LEU
1	C	90	ASP
1	C	97	VAL
1	C	101	ASN
1	C	116	THR
1	C	117	TYR
1	C	123	ILE
1	C	124	ILE
1	C	170	CYS
1	C	273	TRP
2	D	67	TYR
2	D	68	THR
2	D	70	PHE
2	D	90	PRO
1	E	22	ILE
1	E	45	GLN
1	E	72	LEU
1	E	77	LEU
1	E	90	ASP
1	E	97	VAL
1	E	101	ASN
1	E	116	THR
1	E	117	TYR
1	E	123	ILE
1	E	124	ILE
1	E	170	CYS
1	E	273	TRP
2	F	67	TYR
2	F	68	THR

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Mol	Chain	Res	Type
2	F	70	PHE
2	F	90	PRO
1	G	22	ILE
1	G	45	GLN
1	G	72	LEU
1	G	77	LEU
1	G	90	ASP
1	G	97	VAL
1	G	101	ASN
1	G	116	THR
1	G	117	TYR
1	G	123	ILE
1	G	124	ILE
1	G	170	CYS
1	G	273	TRP
2	H	67	TYR
2	H	68	THR
2	H	70	PHE
2	H	90	PRO
1	I	22	ILE
1	I	45	GLN
1	I	72	LEU
1	I	77	LEU
1	I	90	ASP
1	I	97	VAL
1	I	101	ASN
1	I	116	THR
1	I	117	TYR
1	I	123	ILE
1	I	124	ILE
1	I	170	CYS
1	I	273	TRP
2	J	67	TYR
2	J	68	THR
2	J	70	PHE
2	J	90	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	86	ASN
1	A	95	GLN

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Mol	Chain	Res	Type
1	A	104	HIS
1	A	126	ASN
2	B	2	GLN
1	C	86	ASN
1	C	95	GLN
1	C	104	HIS
1	C	126	ASN
2	D	2	GLN
1	E	86	ASN
1	E	95	GLN
1	E	104	HIS
1	E	126	ASN
2	F	2	GLN
1	G	86	ASN
1	G	95	GLN
1	G	104	HIS
1	G	126	ASN
2	H	2	GLN
1	I	86	ASN
1	I	95	GLN
1	I	104	HIS
1	I	126	ASN
1	I	187	HIS
2	J	2	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

### 5.6 Ligand geometry ⓘ

5 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	C	302	1	14,14,15	0.90	1 (7%)	17,19,21	0.75	1 (5%)
3	NAG	I	305	1	14,14,15	0.91	1 (7%)	17,19,21	0.75	1 (5%)
3	NAG	G	304	1	14,14,15	0.90	1 (7%)	17,19,21	0.74	1 (5%)
3	NAG	E	303	1	14,14,15	0.90	1 (7%)	17,19,21	0.74	1 (5%)
3	NAG	A	301	1	14,14,15	0.90	1 (7%)	17,19,21	0.75	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
3	NAG	C	302	1	-	5/6/23/26	0/1/1/1
3	NAG	I	305	1	-	5/6/23/26	0/1/1/1
3	NAG	G	304	1	-	5/6/23/26	0/1/1/1
3	NAG	E	303	1	-	5/6/23/26	0/1/1/1
3	NAG	A	301	1	-	5/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	301	NAG	C1-C2	2.39	1.55	1.52
3	G	304	NAG	C1-C2	2.38	1.55	1.52
3	C	302	NAG	C1-C2	2.38	1.55	1.52
3	I	305	NAG	C1-C2	2.38	1.55	1.52
3	E	303	NAG	C1-C2	2.35	1.55	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	301	NAG	C2-N2-C7	-2.24	119.72	122.90
3	I	305	NAG	C2-N2-C7	-2.23	119.73	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	302	NAG	C2-N2-C7	-2.23	119.73	122.90
3	G	304	NAG	C2-N2-C7	-2.21	119.75	122.90
3	E	303	NAG	C2-N2-C7	-2.20	119.77	122.90

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	302	NAG	C3-C2-N2-C7
3	C	302	NAG	C8-C7-N2-C2
3	C	302	NAG	O7-C7-N2-C2
3	I	305	NAG	C3-C2-N2-C7
3	I	305	NAG	C8-C7-N2-C2
3	I	305	NAG	O7-C7-N2-C2
3	G	304	NAG	C3-C2-N2-C7
3	G	304	NAG	C8-C7-N2-C2
3	G	304	NAG	O7-C7-N2-C2
3	E	303	NAG	C3-C2-N2-C7
3	E	303	NAG	C8-C7-N2-C2
3	E	303	NAG	O7-C7-N2-C2
3	A	301	NAG	C3-C2-N2-C7
3	A	301	NAG	C8-C7-N2-C2
3	A	301	NAG	O7-C7-N2-C2
3	C	302	NAG	O5-C5-C6-O6
3	I	305	NAG	O5-C5-C6-O6
3	G	304	NAG	O5-C5-C6-O6
3	E	303	NAG	O5-C5-C6-O6
3	A	301	NAG	O5-C5-C6-O6
3	C	302	NAG	C4-C5-C6-O6
3	I	305	NAG	C4-C5-C6-O6
3	G	304	NAG	C4-C5-C6-O6
3	E	303	NAG	C4-C5-C6-O6
3	A	301	NAG	C4-C5-C6-O6

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	302	NAG	1	0
3	I	305	NAG	1	0
3	G	304	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	303	NAG	1	0
3	A	301	NAG	2	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	A	261/274 (95%)	0.21	9 (3%)	45	19	17, 54, 112, 167	0
1	C	261/274 (95%)	0.19	7 (2%)	54	26	17, 54, 112, 167	0
1	E	261/274 (95%)	0.20	9 (3%)	45	19	17, 54, 112, 167	0
1	G	261/274 (95%)	-0.02	5 (1%)	66	37	17, 54, 112, 167	0
1	I	261/274 (95%)	0.15	8 (3%)	49	21	17, 54, 112, 167	0
2	B	99/99 (100%)	0.10	1 (1%)	82	59	19, 54, 96, 120	0
2	D	99/99 (100%)	0.02	1 (1%)	82	59	19, 54, 96, 120	0
2	F	99/99 (100%)	0.06	4 (4%)	38	15	19, 54, 96, 120	0
2	H	99/99 (100%)	-0.22	0	100	100	19, 54, 96, 120	0
2	J	99/99 (100%)	0.02	2 (2%)	65	36	19, 54, 96, 120	0
All	All	1800/1865 (96%)	0.10	46 (2%)	56	27	17, 54, 110, 167	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	273	TRP	5.9
1	A	223	HIS	4.7
1	I	253	GLU	4.4
1	I	252	GLU	4.1
1	A	228	GLU	4.0
1	C	227	MET	4.0
1	A	226	ASP	3.9
2	B	99	MET	3.6
1	G	228	GLU	3.6
2	D	42	ASN	3.6
1	C	222	ASN	3.5
1	I	248	VAL	3.4
1	A	251	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
2	F	99	MET	3.3
1	I	199	THR	3.2
1	I	256	TYR	3.2
1	I	247	VAL	3.1
1	G	248	VAL	3.1
1	G	227	MET	3.0
1	C	223	HIS	2.8
2	F	15	ALA	2.8
1	C	228	GLU	2.8
1	C	105	ASP	2.8
1	G	231	ASP	2.7
1	C	215	THR	2.7
1	E	228	GLU	2.5
1	E	110	GLY	2.5
1	E	251	GLY	2.5
1	C	267	GLY	2.5
1	E	245	ALA	2.5
1	A	227	MET	2.4
1	G	256	TYR	2.3
2	F	97	ARG	2.3
2	F	21	ASN	2.3
1	A	246	VAL	2.2
1	A	128	ASP	2.2
1	E	221	LYS	2.2
1	E	193	THR	2.2
1	A	257	THR	2.2
1	A	143	ASN	2.1
1	E	265	LEU	2.1
2	J	90	PRO	2.1
1	I	257	THR	2.1
1	E	222	ASN	2.0
1	E	43	GLY	2.0
2	J	91	LYS	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no monosaccharides 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(Å <sup>2</sup> )	Q<0.9
3	NAG	E	303	14/15	-0.06	0.49	142,142,142,142	0
3	NAG	C	302	14/15	0.21	0.61	142,142,142,142	0
3	NAG	A	301	14/15	0.62	0.31	142,142,142,142	0
3	NAG	I	305	14/15	0.67	0.30	142,142,142,142	0
3	NAG	G	304	14/15	0.68	0.30	142,142,142,142	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.