



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 23, 2018 – 09:32 AM EST

PDB ID : 4WJG  
Title : Structure of T. brucei haptoglobin-hemoglobin receptor binding to human haptoglobin-hemoglobin  
Authors : Støedkilde, K.; Torvund-Jensen, M.; Moestrup, S.K.; Andersen, C.B.F.  
Deposited on : 2014-09-30  
Resolution : 3.10 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-20030736  
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-20030736

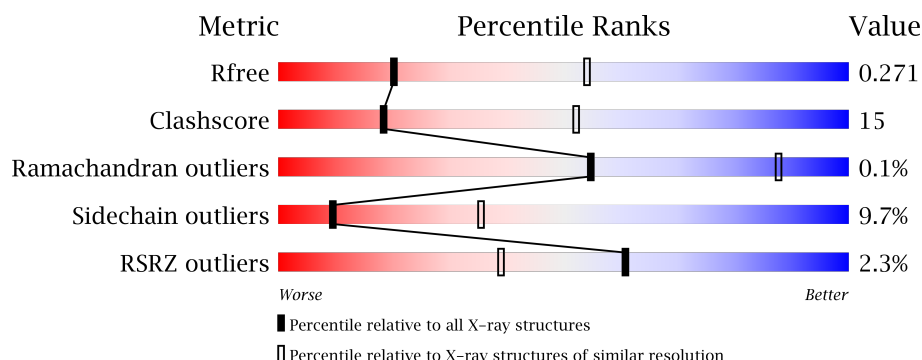
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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	1001 (3.12-3.08)
Clashscore	112137	1099 (3.12-3.08)
Ramachandran outliers	110173	1057 (3.12-3.08)
Sidechain outliers	110143	1057 (3.12-3.08)
RSRZ outliers	101464	1006 (3.12-3.08)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	141	<div> <div>67%</div> <div>28%</div> <div>.</div> </div>
1	F	141	<div> <div>70%</div> <div>26%</div> <div>.</div> </div>
1	K	141	<div> <div>68%</div> <div>28%</div> <div>.</div> </div>
1	P	141	<div> <div>70%</div> <div>27%</div> <div>.</div> </div>
1	U	141	<div> <div>67%</div> <div>29%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	Z	141	
2	1	146	
2	B	146	
2	G	146	
2	L	146	
2	Q	146	
2	V	146	
3	2	315	
3	C	315	
3	H	315	
3	M	315	
3	R	315	
3	W	315	
4	3	146	
4	D	146	
4	I	146	
4	N	146	
4	S	146	
4	X	146	
5	4	343	
5	E	343	
5	J	343	
5	O	343	
5	T	343	
5	Y	343	

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 47792 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 Hemoglobin subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	141	Total	C	N	O	S	0	0	0
			1069	685	187	194	3			
1	F	141	Total	C	N	O	S	0	0	0
			1069	685	187	194	3			
1	K	141	Total	C	N	O	S	0	0	0
			1069	685	187	194	3			
1	P	141	Total	C	N	O	S	0	0	0
			1069	685	187	194	3			
1	U	141	Total	C	N	O	S	0	0	0
			1069	685	187	194	3			
1	Z	141	Total	C	N	O	S	0	0	0
			1069	685	187	194	3			

- Molecule 2 is a protein called Hemoglobin subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	146	Total	C	N	O	S	0	0	0
			1123	724	195	201	3			
2	G	146	Total	C	N	O	S	0	0	0
			1123	724	195	201	3			
2	L	146	Total	C	N	O	S	0	0	0
			1123	724	195	201	3			
2	Q	146	Total	C	N	O	S	0	0	0
			1123	724	195	201	3			
2	V	146	Total	C	N	O	S	0	0	0
			1123	724	195	201	3			
2	1	146	Total	C	N	O	S	0	0	0
			1123	724	195	201	3			

- Molecule 3 is a protein called Haptoglobin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	310	Total	C	N	O	S	0	0	0
			2437	1552	413	459	13			
3	H	310	Total	C	N	O	S	0	0	0
			2437	1552	413	459	13			
3	M	310	Total	C	N	O	S	0	0	0
			2437	1552	413	459	13			
3	R	310	Total	C	N	O	S	0	0	0
			2437	1552	413	459	13			
3	W	310	Total	C	N	O	S	0	0	0
			2437	1552	413	459	13			
3	2	310	Total	C	N	O	S	0	0	0
			2437	1552	413	459	13			

- Molecule 4 is a protein called Iron-regulated surface determinant protein H.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	144	Total	C	N	O	0	0	0
			1183	754	189	240			
4	I	144	Total	C	N	O	0	0	0
			1183	754	189	240			
4	N	144	Total	C	N	O	0	0	0
			1183	754	189	240			
4	S	144	Total	C	N	O	0	0	0
			1183	754	189	240			
4	X	144	Total	C	N	O	0	0	0
			1183	754	189	240			
4	3	144	Total	C	N	O	0	0	0
			1183	754	189	240			

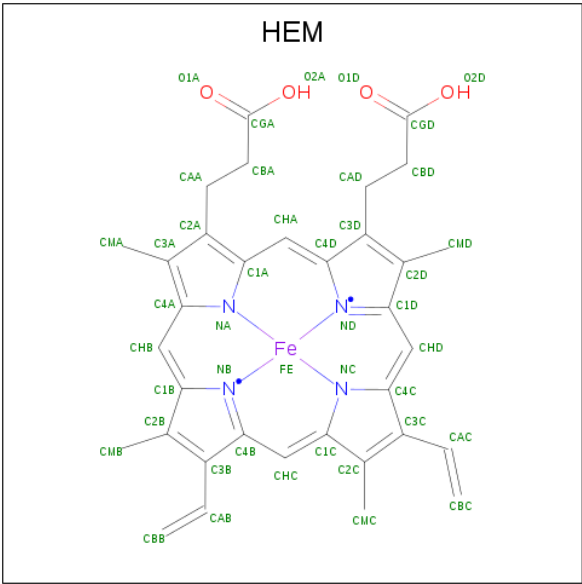
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	84	GLY	-	expression tag	UNP Q99TD3
D	85	SER	-	expression tag	UNP Q99TD3
I	84	GLY	-	expression tag	UNP Q99TD3
I	85	SER	-	expression tag	UNP Q99TD3
N	84	GLY	-	expression tag	UNP Q99TD3
N	85	SER	-	expression tag	UNP Q99TD3
S	84	GLY	-	expression tag	UNP Q99TD3
S	85	SER	-	expression tag	UNP Q99TD3
X	84	GLY	-	expression tag	UNP Q99TD3
X	85	SER	-	expression tag	UNP Q99TD3
3	84	GLY	-	expression tag	UNP Q99TD3
3	85	SER	-	expression tag	UNP Q99TD3

- Molecule 5 is a protein called Haptoglobin-hemoglobin receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	261	Total	C	N	O	S	0	0	0
			1963	1202	365	393	3			
5	J	261	Total	C	N	O	S	0	0	0
			1963	1202	365	393	3			
5	O	261	Total	C	N	O	S	0	0	0
			1963	1202	365	393	3			
5	T	261	Total	C	N	O	S	0	0	0
			1963	1202	365	393	3			
5	Y	261	Total	C	N	O	S	0	0	0
			1963	1202	365	393	3			
5	4	261	Total	C	N	O	S	0	0	0
			1963	1202	365	393	3			

- Molecule 6 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).



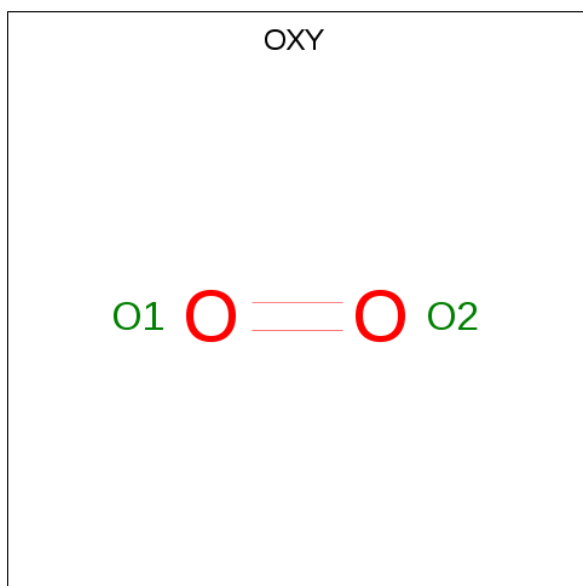
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
6	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
6	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
6	G	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	K	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	L	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	P	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	Q	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	U	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	V	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	Z	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
6	1	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 7 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O<sub>2</sub>).



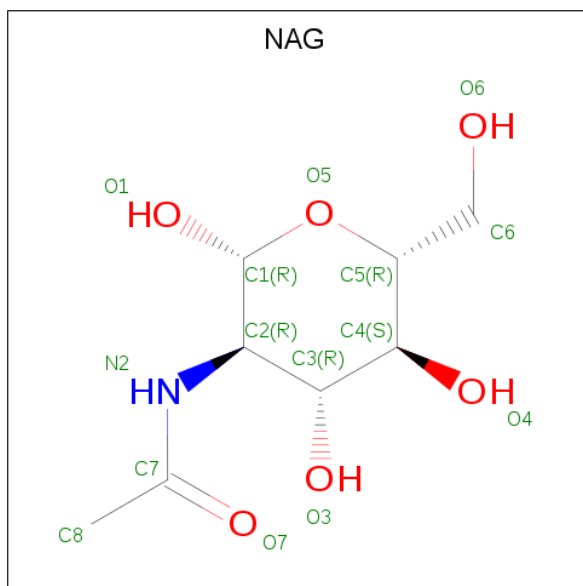
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total 2	O 2	0	0
7	B	1	Total 2	O 2	0	0
7	F	1	Total 2	O 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	G	1	Total	O	0	0
			2	2		
7	K	1	Total	O	0	0
			2	2		
7	L	1	Total	O	0	0
			2	2		
7	P	1	Total	O	0	0
			2	2		
7	Q	1	Total	O	0	0
			2	2		
7	U	1	Total	O	0	0
			2	2		
7	V	1	Total	O	0	0
			2	2		
7	Z	1	Total	O	0	0
			2	2		
7	1	1	Total	O	0	0
			2	2		

- Molecule 8 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
8	C	1	Total	C	N	O	0	0
			14	8	1	5		
8	C	1	Total	C	N	O	0	0
			14	8	1	5		

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

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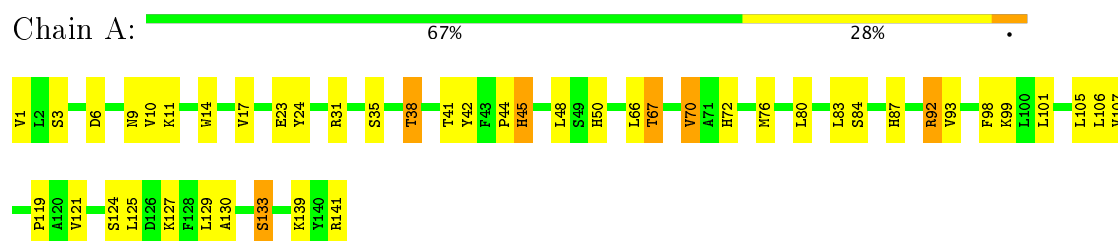
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	R	1	Total	C	N	O	0	0
			14	8	1	5		
8	R	1	Total	C	N	O	0	0
			14	8	1	5		
8	R	1	Total	C	N	O	0	0
			14	8	1	5		
8	R	1	Total	C	N	O	0	0
			14	8	1	5		
8	R	1	Total	C	N	O	0	0
			14	8	1	5		
8	T	1	Total	C	N	O	0	0
			14	8	1	5		
8	T	1	Total	C	N	O	0	0
			14	8	1	5		
8	W	1	Total	C	N	O	0	0
			14	8	1	5		
8	W	1	Total	C	N	O	0	0
			14	8	1	5		
8	W	1	Total	C	N	O	0	0
			14	8	1	5		
8	W	1	Total	C	N	O	0	0
			14	8	1	5		
8	Y	1	Total	C	N	O	0	0
			14	8	1	5		
8	Y	1	Total	C	N	O	0	0
			14	8	1	5		
8	2	1	Total	C	N	O	0	0
			14	8	1	5		
8	2	1	Total	C	N	O	0	0
			14	8	1	5		
8	2	1	Total	C	N	O	0	0
			14	8	1	5		
8	2	1	Total	C	N	O	0	0
			14	8	1	5		
8	4	1	Total	C	N	O	0	0
			14	8	1	5		
8	4	1	Total	C	N	O	0	0
			14	8	1	5		

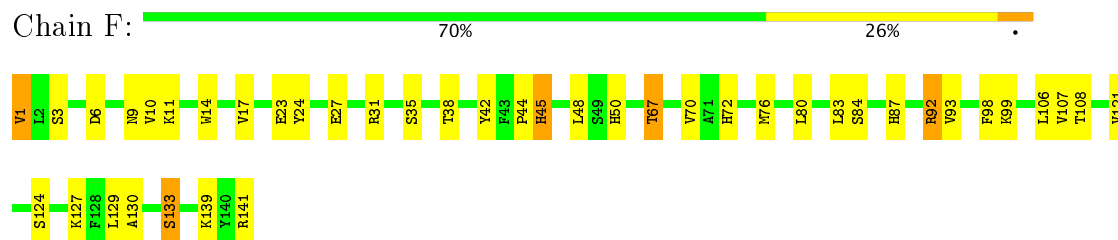
### 3 Residue-property plots

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

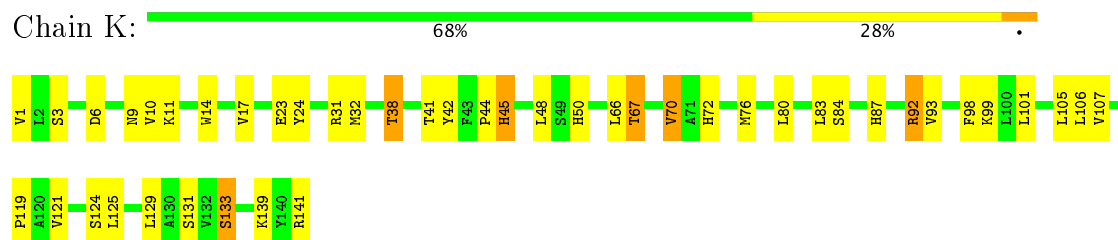
- Molecule 1: Hemoglobin subunit alpha



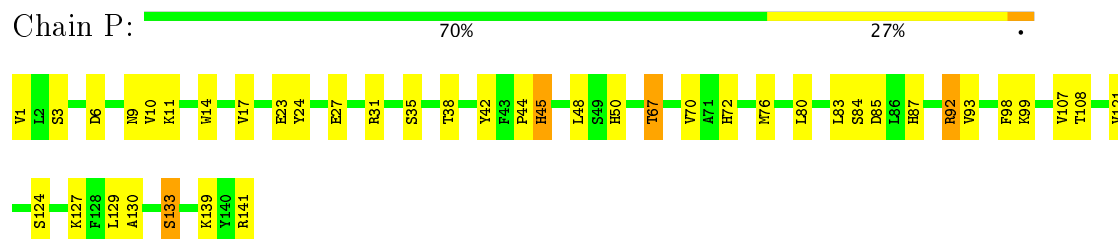
- Molecule 1: Hemoglobin subunit alpha



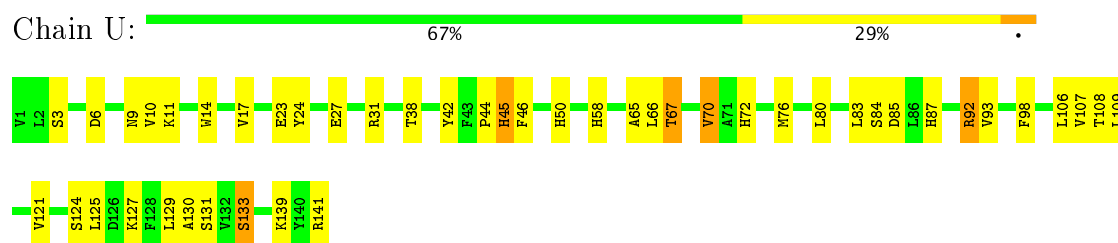
- Molecule 1: Hemoglobin subunit alpha



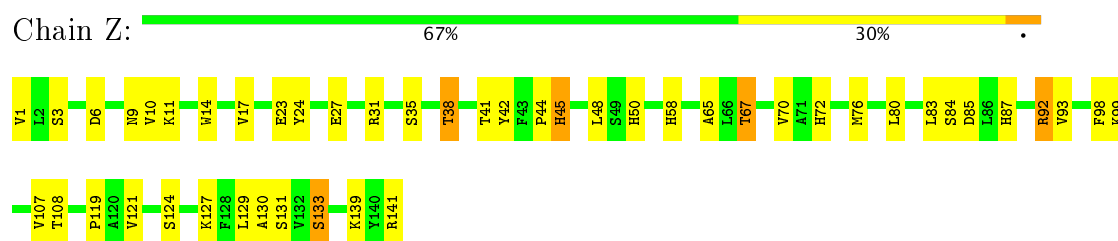
- Molecule 1: Hemoglobin subunit alpha



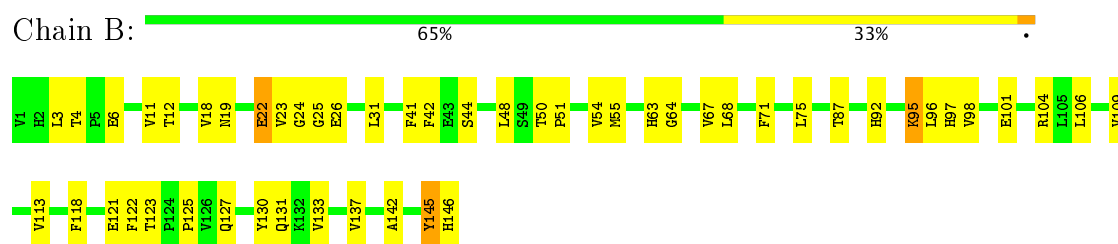
- Molecule 1: Hemoglobin subunit alpha



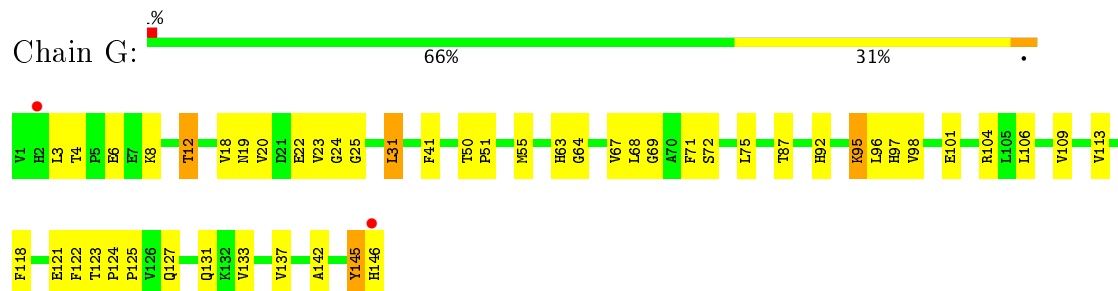
- Molecule 1: Hemoglobin subunit alpha



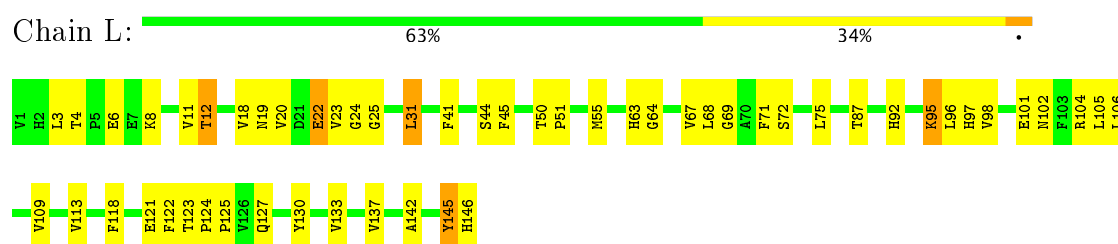
- Molecule 2: Hemoglobin subunit beta



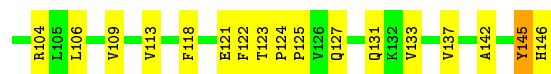
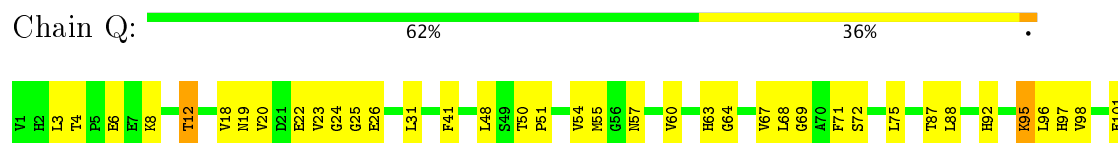
- Molecule 2: Hemoglobin subunit beta



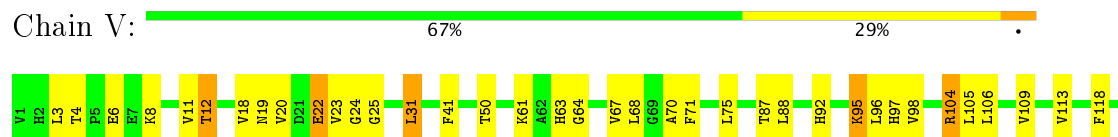
- Molecule 2: Hemoglobin subunit beta



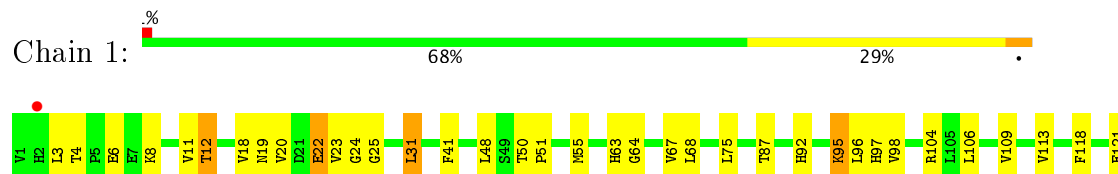
- Molecule 2: Hemoglobin subunit beta



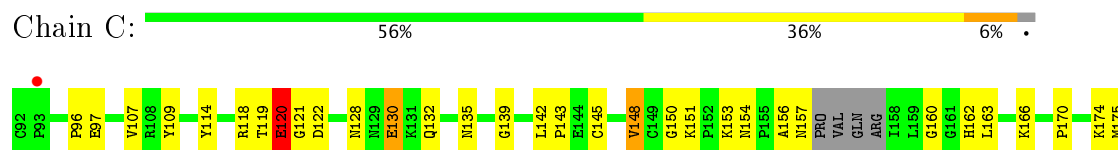
• Molecule 2: Hemoglobin subunit beta



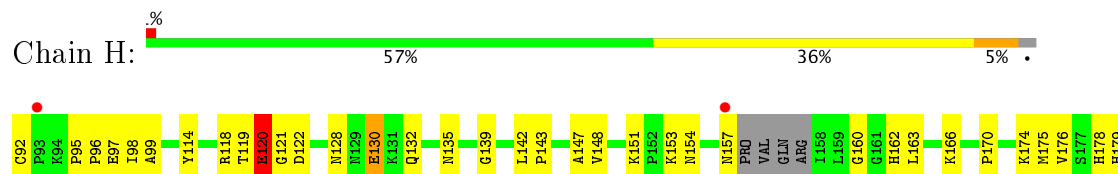
• Molecule 2: Hemoglobin subunit beta

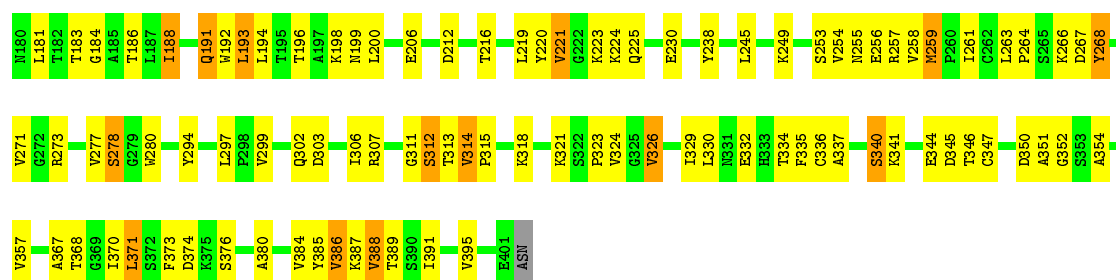


• Molecule 3: Haptoglobin



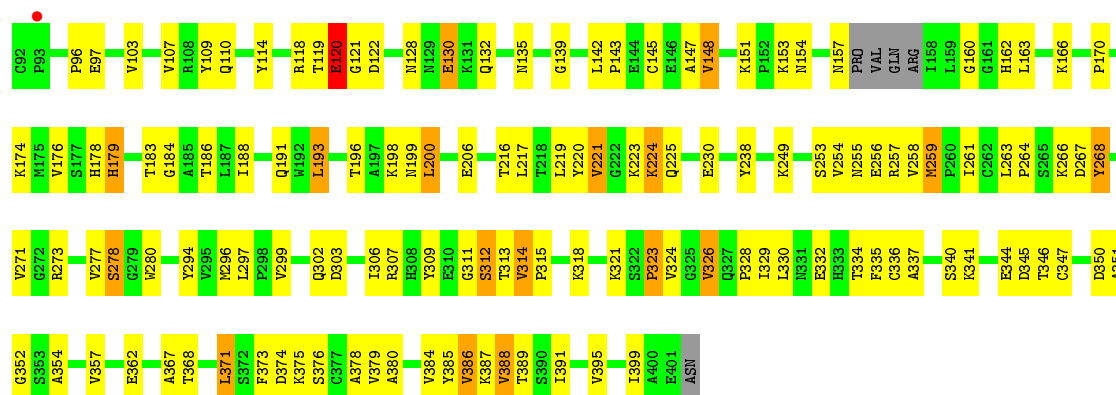
• Molecule 3: Haptoglobin





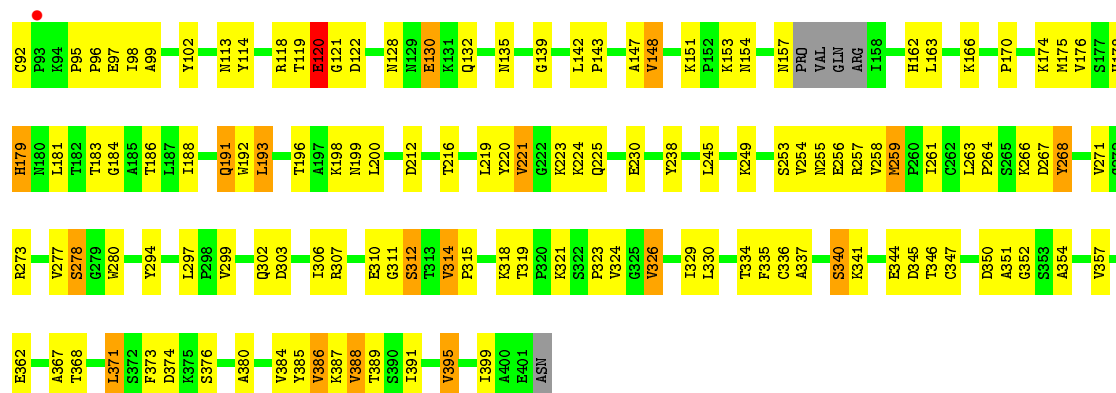
• Molecule 3: Haptoglobin

Chain M: 56% 37% 5% .



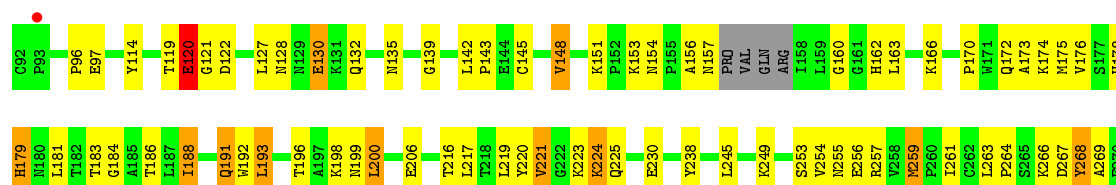
• Molecule 3: Haptoglobin

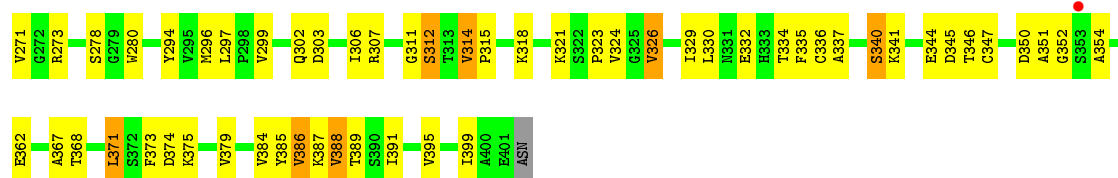
Chain R: 57% 36% 5% .



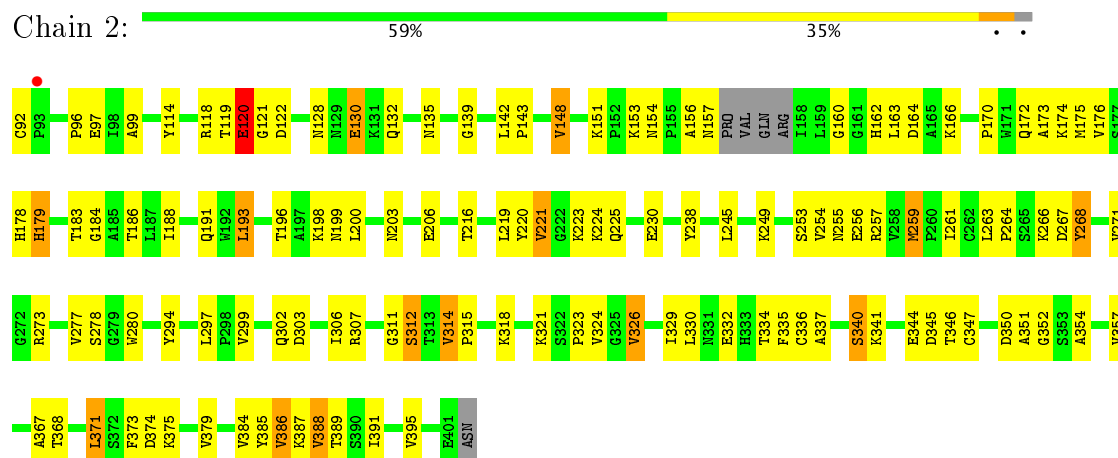
• Molecule 3: Haptoglobin

Chain W: 58% 34% 6% .

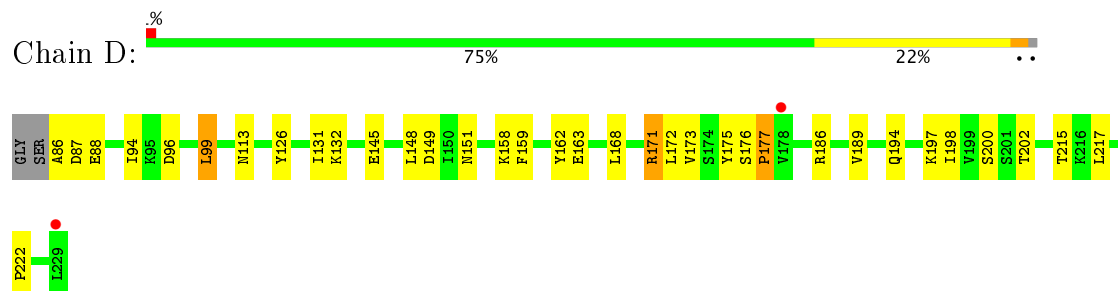




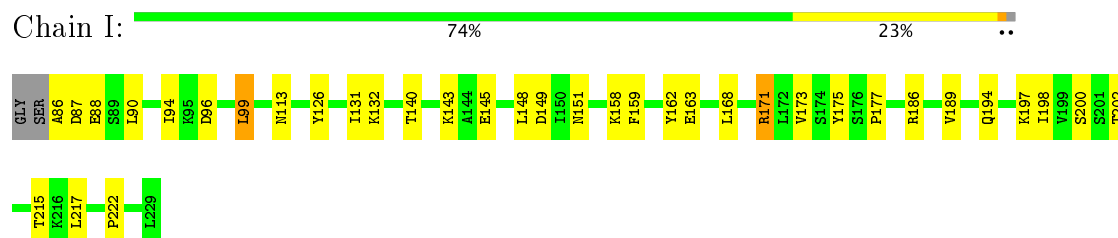
• Molecule 3: Haptoglobin



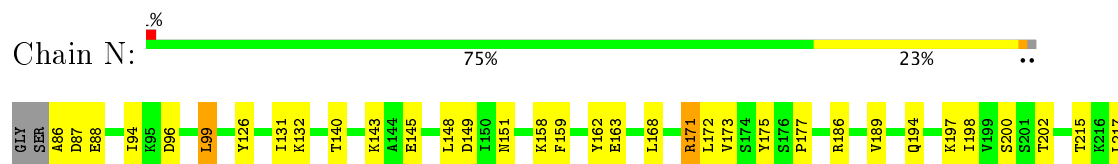
• Molecule 4: Iron-regulated surface determinant protein H



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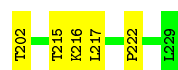
• Molecule 4: Iron-regulated surface determinant protein H





- Molecule 4: Iron-regulated surface determinant protein H

Chain S: 73% 25% ..



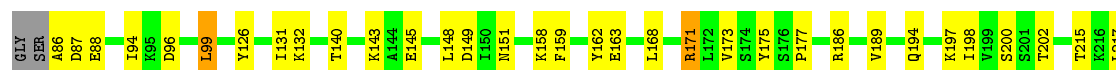
- Molecule 4: Iron-regulated surface determinant protein H

Chain X: 75% 22% ..



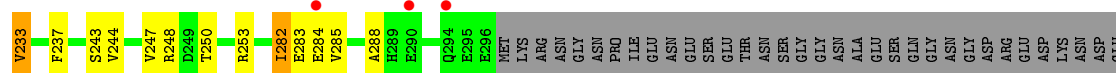
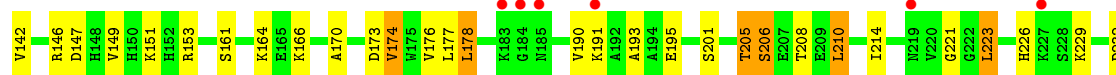
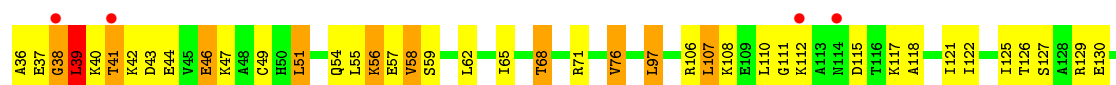
- Molecule 4: Iron-regulated surface determinant protein H

Chain 3: 75% 22% ..



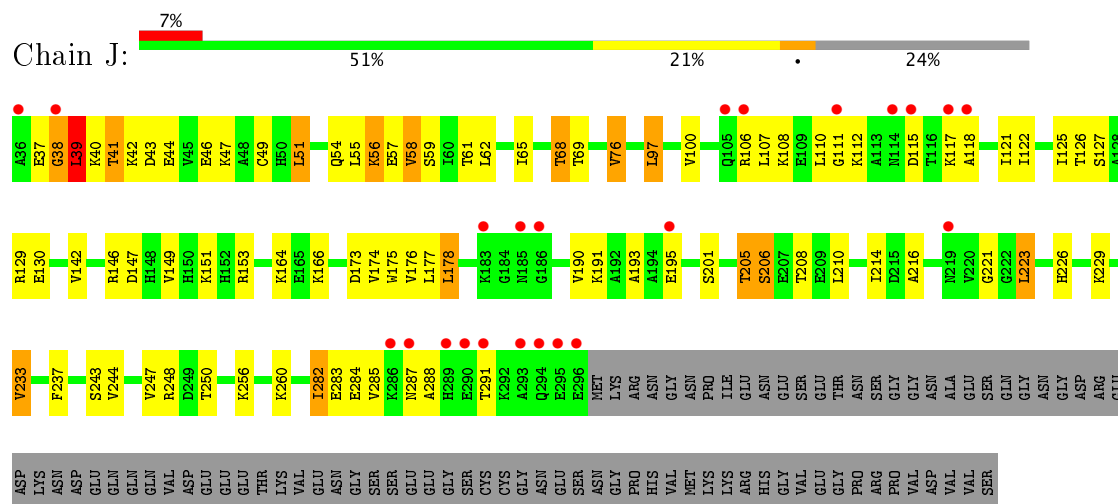
- Molecule 5: Haptoglobin-hemoglobin receptor

Chain E: 4% 52% 19% 5% 24%

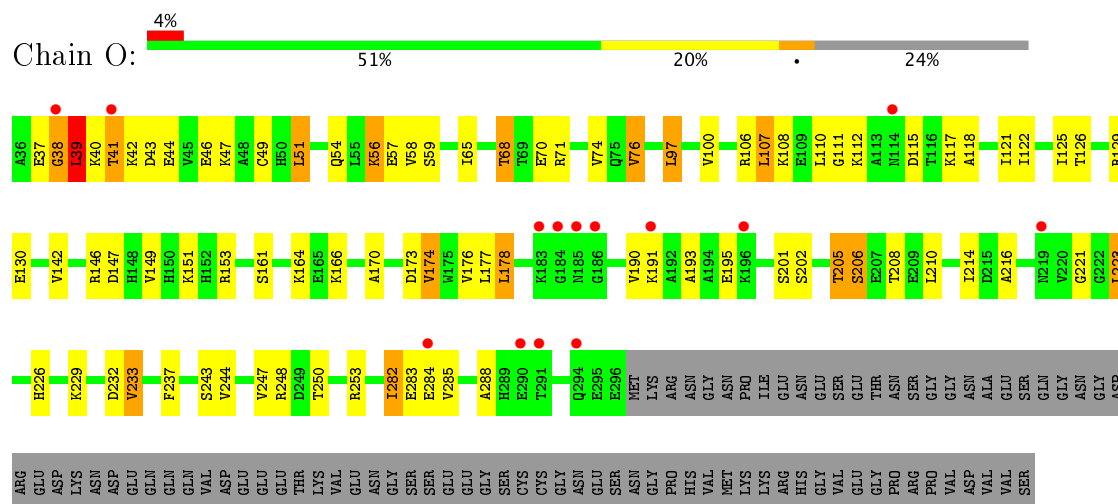




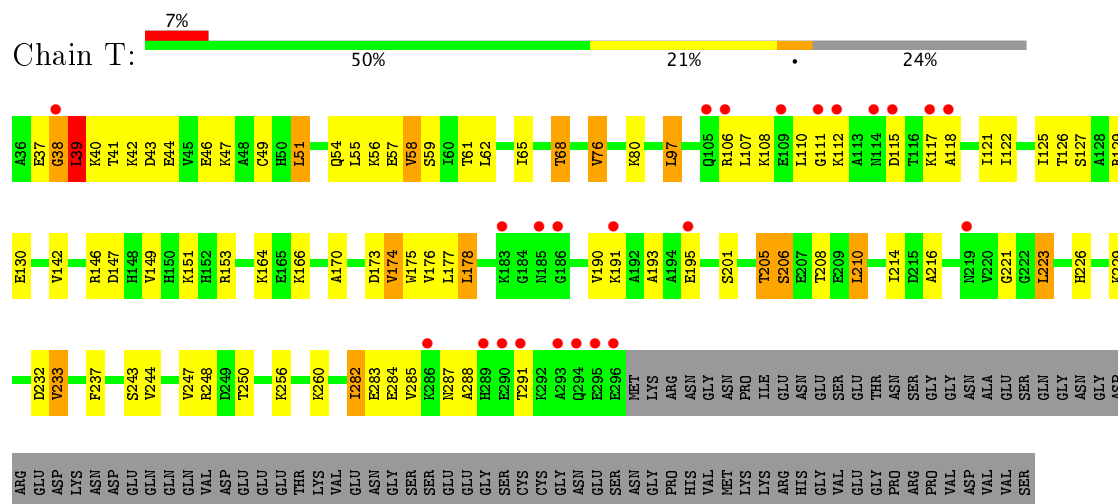
- Molecule 5: Haptoglobin-hemoglobin receptor



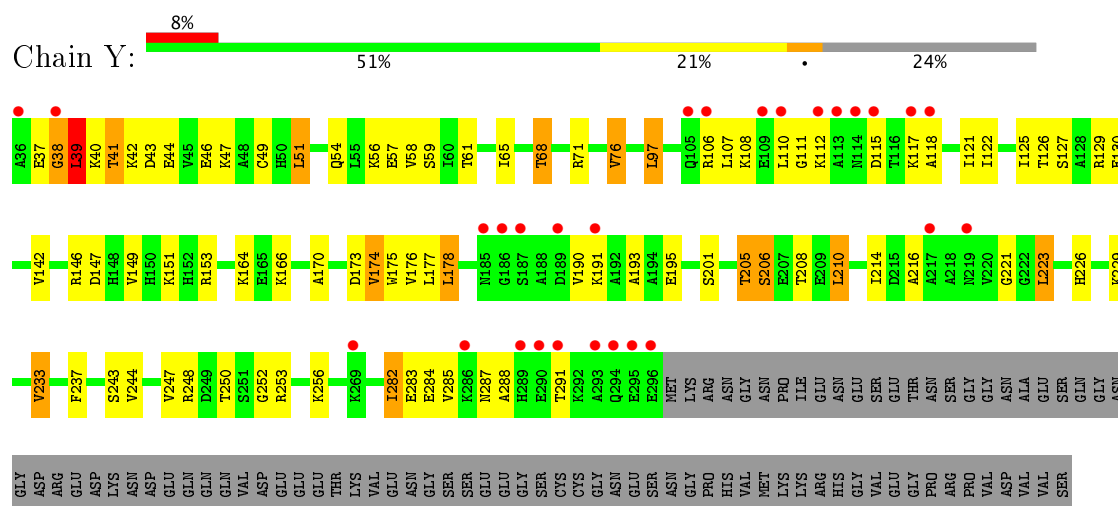
- Molecule 5: Haptoglobin-hemoglobin receptor



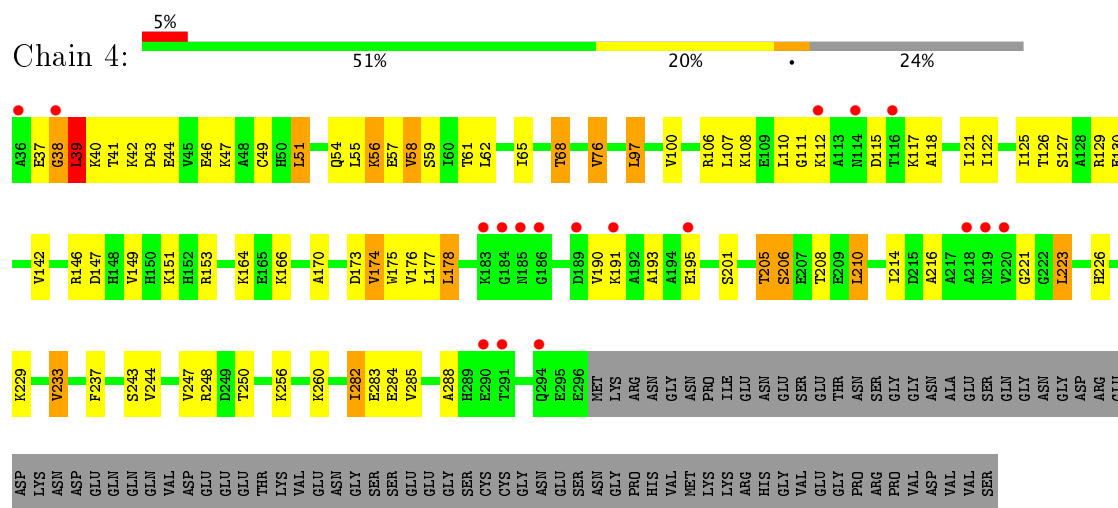
- Molecule 5: Haptoglobin-hemoglobin receptor



- Molecule 5: Haptoglobin-hemoglobin receptor



• Molecule 5: Haptoglobin-hemoglobin receptor



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	143.23Å 140.95Å 267.18Å 90.00° 98.54° 90.00°	Depositor
Resolution (Å)	29.00 – 3.10 28.98 – 3.10	Depositor EDS
% Data completeness (in resolution range)	96.1 (29.00-3.10) 96.7 (28.98-3.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.80 (at 3.11Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1702)	Depositor
R, $R_{free}$	0.255 , 0.271 0.255 , 0.271	Depositor DCC
$R_{free}$ test set	1756 reflections (0.96%)	DCC
Wilson B-factor (Å <sup>2</sup> )	65.7	Xtriage
Anisotropy	0.870	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 38.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	47792	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 53.03 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 4.4672e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: HEM, NAG, OXY

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	0.54	0/1097	0.66	0/1491
1	F	0.52	0/1097	0.69	2/1491 (0.1%)
1	K	0.54	0/1097	0.68	0/1491
1	P	0.51	0/1097	0.64	0/1491
1	U	0.46	0/1097	0.61	0/1491
1	Z	0.47	0/1097	0.61	0/1491
2	1	0.49	0/1153	0.61	0/1566
2	B	0.59	0/1153	0.67	0/1566
2	G	0.57	0/1153	0.65	0/1566
2	L	0.59	0/1153	0.68	0/1566
2	Q	0.56	0/1153	0.65	0/1566
2	V	0.51	0/1153	0.61	0/1566
3	2	0.52	0/2497	0.71	0/3391
3	C	0.64	0/2497	0.77	0/3391
3	H	0.57	0/2497	0.74	0/3391
3	M	0.64	0/2497	0.77	0/3391
3	R	0.57	0/2497	0.74	0/3391
3	W	0.49	0/2497	0.71	0/3391
4	3	0.44	0/1212	0.62	0/1647
4	D	0.51	0/1212	0.66	0/1647
4	I	0.49	0/1212	0.65	0/1647
4	N	0.52	0/1212	0.66	0/1647
4	S	0.49	0/1212	0.65	0/1647
4	X	0.43	0/1212	0.63	0/1647
5	4	0.41	0/1981	0.62	1/2666 (0.0%)
5	E	0.45	0/1981	0.63	1/2666 (0.0%)
5	J	0.42	0/1981	0.62	1/2666 (0.0%)
5	O	0.48	0/1981	0.64	1/2666 (0.0%)
5	T	0.42	0/1981	0.62	1/2666 (0.0%)
5	Y	0.39	0/1981	0.61	1/2666 (0.0%)
All	All	0.52	0/47640	0.67	8/64566 (0.0%)

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
3	2	0	3
3	C	0	4
3	H	0	3
3	M	0	4
3	R	0	3
3	W	0	3
4	3	0	1
4	D	0	1
4	I	0	1
4	N	0	1
4	S	0	1
4	X	0	1
5	4	0	1
5	E	0	1
5	J	0	1
5	O	0	1
5	T	0	1
5	Y	0	1
All	All	0	32

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	1	VAL	CG1-CB-CG2	6.10	120.66	110.90
1	F	1	VAL	CB-CA-C	-5.41	101.12	111.40
5	E	223	LEU	CA-CB-CG	5.25	127.38	115.30
5	T	223	LEU	CA-CB-CG	5.12	127.07	115.30
5	4	223	LEU	CA-CB-CG	5.09	127.01	115.30
5	Y	223	LEU	CA-CB-CG	5.08	126.98	115.30
5	O	223	LEU	CA-CB-CG	5.07	126.97	115.30
5	J	223	LEU	CA-CB-CG	5.06	126.94	115.30

There are no chirality outliers.

All (32) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	2	120	GLU	Peptide
3	2	311	GLY	Peptide
3	2	312	SER	Peptide
4	3	177	PRO	Peptide
5	4	38	GLY	Peptide
3	C	120	GLU	Peptide
3	C	311	GLY	Peptide
3	C	312	SER	Peptide
3	C	378	ALA	Peptide
4	D	177	PRO	Peptide
5	E	38	GLY	Peptide
3	H	120	GLU	Peptide
3	H	311	GLY	Peptide
3	H	312	SER	Peptide
4	I	177	PRO	Peptide
5	J	38	GLY	Peptide
3	M	120	GLU	Peptide
3	M	311	GLY	Peptide
3	M	312	SER	Peptide
3	M	378	ALA	Peptide
4	N	177	PRO	Peptide
5	O	38	GLY	Peptide
3	R	120	GLU	Peptide
3	R	311	GLY	Peptide
3	R	312	SER	Peptide
4	S	177	PRO	Peptide
5	T	38	GLY	Peptide
3	W	120	GLU	Peptide
3	W	311	GLY	Peptide
3	W	312	SER	Peptide
4	X	177	PRO	Peptide
5	Y	38	GLY	Peptide

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1069	0	1073	30	0
1	F	1069	0	1073	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	K	1069	0	1073	30	0
1	P	1069	0	1073	24	0
1	U	1069	0	1073	33	0
1	Z	1069	0	1073	31	0
2	1	1123	0	1118	32	0
2	B	1123	0	1118	37	0
2	G	1123	0	1118	30	0
2	L	1123	0	1118	39	0
2	Q	1123	0	1118	34	0
2	V	1123	0	1118	33	0
3	2	2437	0	2388	96	0
3	C	2437	0	2387	104	0
3	H	2437	0	2388	100	0
3	M	2437	0	2387	104	0
3	R	2437	0	2387	103	0
3	W	2437	0	2388	95	0
4	3	1183	0	1132	16	0
4	D	1183	0	1132	19	0
4	I	1183	0	1132	17	0
4	N	1183	0	1132	18	0
4	S	1183	0	1132	17	0
4	X	1183	0	1132	17	0
5	4	1963	0	1978	57	0
5	E	1963	0	1978	65	0
5	J	1963	0	1978	60	0
5	O	1963	0	1978	58	0
5	T	1963	0	1978	58	0
5	Y	1963	0	1978	62	0
6	1	43	0	30	6	0
6	A	43	0	30	1	0
6	B	43	0	30	6	0
6	F	43	0	30	2	0
6	G	43	0	30	3	0
6	K	43	0	30	1	0
6	L	43	0	30	6	0
6	P	43	0	30	2	0
6	Q	43	0	30	4	0
6	U	43	0	30	4	0
6	V	43	0	30	3	0
6	Z	43	0	30	2	0
7	1	2	0	0	0	0
7	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	2	0	0	0	0
7	F	2	0	0	0	0
7	G	2	0	0	0	0
7	K	2	0	0	0	0
7	L	2	0	0	0	0
7	P	2	0	0	0	0
7	Q	2	0	0	0	0
7	U	2	0	0	1	0
7	V	2	0	0	1	0
7	Z	2	0	0	1	0
8	2	70	0	63	3	0
8	4	28	0	26	2	0
8	C	84	0	76	3	0
8	E	28	0	26	1	0
8	H	56	0	51	3	0
8	J	28	0	26	2	0
8	M	84	0	76	4	0
8	O	28	0	26	1	0
8	R	84	0	76	3	0
8	T	28	0	26	1	0
8	W	56	0	51	2	0
8	Y	28	0	26	1	0
All	All	47792	0	47040	1408	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (1408) 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)
5:E:43:ASP:OD2	5:E:47:LYS:HE2	1.30	1.29
5:E:43:ASP:OD2	5:E:47:LYS:CE	2.15	0.94
3:2:183:THR:HB	3:2:199:ASN:HD22	1.36	0.89
3:M:183:THR:HB	3:M:199:ASN:HD22	1.35	0.89
5:O:57:GLU:HG3	5:O:201:SER:HB3	1.55	0.88
5:Y:57:GLU:HG3	5:Y:201:SER:HB3	1.57	0.87
3:C:188:ILE:HD11	3:C:263:LEU:HD21	1.57	0.86
3:C:183:THR:HB	3:C:199:ASN:HD22	1.39	0.86
3:M:188:ILE:HD11	3:M:263:LEU:HD21	1.57	0.85
5:T:57:GLU:HG3	5:T:201:SER:HB3	1.58	0.85
5:4:57:GLU:HG3	5:4:201:SER:HB3	1.57	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:183:THR:HB	3:H:199:ASN:HD22	1.39	0.85
3:R:183:THR:HB	3:R:199:ASN:HD22	1.41	0.84
1:Z:83:LEU:HD22	1:Z:87:HIS:HE1	1.43	0.84
5:J:57:GLU:HG3	5:J:201:SER:HB3	1.59	0.83
3:R:188:ILE:HD11	3:R:263:LEU:HD21	1.59	0.83
3:W:183:THR:HB	3:W:199:ASN:HD22	1.40	0.83
2:L:106:LEU:HD23	6:L:201:HEM:HBB2	1.60	0.83
3:W:188:ILE:HD11	3:W:263:LEU:HD21	1.60	0.83
1:F:83:LEU:HD22	1:F:87:HIS:HE1	1.44	0.83
1:U:83:LEU:HD22	1:U:87:HIS:HE1	1.44	0.82
5:E:57:GLU:HG3	5:E:201:SER:HB3	1.60	0.82
3:W:128:ASN:HB2	3:W:132:GLN:H	1.43	0.82
3:M:373:PHE:HB3	3:M:384:VAL:HG12	1.61	0.82
3:2:188:ILE:HD11	3:2:263:LEU:HD21	1.61	0.82
1:K:83:LEU:HD22	1:K:87:HIS:HE1	1.45	0.82
1:A:83:LEU:HD22	1:A:87:HIS:HE1	1.45	0.81
1:P:83:LEU:HD22	1:P:87:HIS:HE1	1.45	0.81
3:C:373:PHE:HB3	3:C:384:VAL:HG12	1.63	0.81
3:H:188:ILE:HD11	3:H:263:LEU:HD21	1.62	0.80
3:M:128:ASN:HB2	3:M:132:GLN:H	1.45	0.80
6:Q:201:HEM:HBB2	6:Q:201:HEM:HHC	1.62	0.80
3:H:128:ASN:HB2	3:H:132:GLN:H	1.44	0.80
3:2:373:PHE:HB3	3:2:384:VAL:HG12	1.63	0.80
3:C:128:ASN:HB2	3:C:132:GLN:H	1.46	0.80
3:W:373:PHE:HB3	3:W:384:VAL:HG12	1.64	0.80
3:2:128:ASN:HB2	3:2:132:GLN:H	1.45	0.79
5:E:43:ASP:O	5:E:46:GLU:HG3	1.82	0.79
3:R:128:ASN:HB2	3:R:132:GLN:H	1.45	0.78
3:R:373:PHE:HB3	3:R:384:VAL:HG12	1.64	0.78
2:G:24:GLY:H	2:G:68:LEU:HD22	1.50	0.77
5:O:40:LYS:HB3	5:O:44:GLU:HB3	1.64	0.77
1:Z:9:ASN:HD22	1:Z:121:VAL:HG22	1.49	0.77
3:M:268:TYR:HB3	3:M:273:ARG:HG3	1.67	0.77
4:S:132:LYS:HB3	4:S:149:ASP:HB3	1.64	0.77
1:K:9:ASN:HD22	1:K:121:VAL:HG22	1.48	0.77
2:1:24:GLY:H	2:1:68:LEU:HD22	1.50	0.77
5:E:40:LYS:HB3	5:E:44:GLU:HB3	1.65	0.77
3:H:157:ASN:ND2	5:J:68:THR:O	2.18	0.77
5:J:40:LYS:HB3	5:J:44:GLU:HB3	1.64	0.77
3:W:268:TYR:HB3	3:W:273:ARG:HG3	1.67	0.77
5:4:40:LYS:HB3	5:4:44:GLU:HB3	1.64	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:9:ASN:HD22	1:F:121:VAL:HG22	1.50	0.76
4:N:132:LYS:HB3	4:N:149:ASP:HB3	1.67	0.76
5:Y:40:LYS:HB3	5:Y:44:GLU:HB3	1.65	0.76
3:H:373:PHE:HB3	3:H:384:VAL:HG12	1.67	0.76
2:B:24:GLY:H	2:B:68:LEU:HD22	1.50	0.76
2:L:24:GLY:H	2:L:68:LEU:HD22	1.50	0.76
2:V:24:GLY:HA3	2:V:68:LEU:HB2	1.66	0.76
2:G:24:GLY:HA3	2:G:68:LEU:HB2	1.66	0.76
3:H:268:TYR:HB3	3:H:273:ARG:HG3	1.66	0.76
5:T:40:LYS:HB3	5:T:44:GLU:HB3	1.65	0.76
2:V:24:GLY:H	2:V:68:LEU:HD22	1.51	0.75
4:D:132:LYS:HB3	4:D:149:ASP:HB3	1.68	0.75
1:U:9:ASN:HD22	1:U:121:VAL:HG22	1.52	0.75
4:I:132:LYS:HB3	4:I:149:ASP:HB3	1.68	0.75
1:K:101:LEU:HD23	6:K:201:HEM:HBB2	1.69	0.75
2:Q:24:GLY:HA3	2:Q:68:LEU:HB2	1.67	0.75
6:1:201:HEM:HBB2	6:1:201:HEM:HHC	1.69	0.75
4:3:132:LYS:HB3	4:3:149:ASP:HB3	1.68	0.75
3:C:315:PRO:HA	3:C:318:LYS:HG3	1.69	0.75
2:Q:24:GLY:H	2:Q:68:LEU:HD22	1.53	0.74
4:S:162:TYR:HB2	4:S:197:LYS:HB3	1.70	0.74
1:A:9:ASN:HD22	1:A:121:VAL:HG22	1.52	0.74
2:1:24:GLY:HA3	2:1:68:LEU:HB2	1.67	0.74
3:C:268:TYR:HB3	3:C:273:ARG:HG3	1.70	0.74
6:G:201:HEM:HBB2	6:G:201:HEM:HHC	1.68	0.74
5:T:147:ASP:OD2	5:T:151:LYS:NZ	2.19	0.74
4:D:162:TYR:HB2	4:D:197:LYS:HB3	1.68	0.74
5:4:147:ASP:OD2	5:4:151:LYS:NZ	2.19	0.74
4:X:132:LYS:HB3	4:X:149:ASP:HB3	1.68	0.74
2:L:41:PHE:CE2	2:L:98:VAL:HG22	2.23	0.73
4:N:162:TYR:HB2	4:N:197:LYS:HB3	1.69	0.73
1:P:9:ASN:HD22	1:P:121:VAL:HG22	1.53	0.73
3:M:315:PRO:HA	3:M:318:LYS:HG3	1.70	0.73
2:B:41:PHE:CE2	2:B:98:VAL:HG22	2.24	0.73
6:B:201:HEM:HBA2	6:B:201:HEM:HHA	1.71	0.73
2:L:24:GLY:HA3	2:L:68:LEU:HB2	1.68	0.72
5:O:59:SER:HB2	5:O:164:LYS:HG3	1.70	0.72
3:2:268:TYR:HB3	3:2:273:ARG:HG3	1.70	0.72
5:E:59:SER:HB2	5:E:164:LYS:HG3	1.70	0.72
4:3:162:TYR:HB2	4:3:197:LYS:HB3	1.72	0.72
4:I:162:TYR:HB2	4:I:197:LYS:HB3	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:261:ILE:HD13	3:C:367:ALA:HB2	1.72	0.72
3:R:268:TYR:HB3	3:R:273:ARG:HG3	1.70	0.72
3:C:178:HIS:HB2	3:C:216:THR:HG23	1.72	0.71
5:Y:147:ASP:OD2	5:Y:151:LYS:NZ	2.19	0.71
2:B:24:GLY:HA3	2:B:68:LEU:HB2	1.69	0.71
8:R:1006:NAG:O3	8:R:1006:NAG:O7	2.09	0.71
5:4:59:SER:HB2	5:4:164:LYS:HG3	1.72	0.71
4:X:162:TYR:HB2	4:X:197:LYS:HB3	1.72	0.71
3:2:178:HIS:HB2	3:2:216:THR:HG23	1.71	0.71
3:M:178:HIS:HB2	3:M:216:THR:HG23	1.72	0.70
3:H:315:PRO:HA	3:H:318:LYS:HG3	1.71	0.70
5:T:256:LYS:HE3	5:T:260:LYS:HE3	1.74	0.70
3:R:178:HIS:HB2	3:R:216:THR:HG23	1.72	0.70
3:R:315:PRO:HA	3:R:318:LYS:HG3	1.72	0.70
5:E:54:GLN:HE21	5:E:205:THR:HG23	1.57	0.69
3:W:315:PRO:HA	3:W:318:LYS:HG3	1.74	0.69
3:H:178:HIS:HB2	3:H:216:THR:HG23	1.73	0.69
5:T:247:VAL:HA	5:T:250:THR:HG22	1.75	0.69
2:B:41:PHE:HE2	2:B:98:VAL:HG22	1.57	0.69
2:L:41:PHE:HE2	2:L:98:VAL:HG22	1.56	0.69
3:M:261:ILE:HD13	3:M:367:ALA:HB2	1.74	0.69
3:M:196:THR:OG1	3:M:199:ASN:OD1	2.08	0.69
3:R:193:LEU:HD13	3:R:219:LEU:HD21	1.73	0.69
3:2:315:PRO:HA	3:2:318:LYS:HG3	1.73	0.69
6:B:201:HEM:HHC	6:B:201:HEM:HBB2	1.75	0.69
5:O:54:GLN:HE21	5:O:205:THR:HG23	1.58	0.68
4:S:86:ALA:N	4:S:88:GLU:OE2	2.26	0.68
3:W:178:HIS:HB2	3:W:216:THR:HG23	1.74	0.68
3:M:193:LEU:HD13	3:M:219:LEU:HD21	1.76	0.68
5:4:247:VAL:HA	5:4:250:THR:HG22	1.76	0.68
3:C:193:LEU:HD13	3:C:219:LEU:HD21	1.76	0.68
1:K:42:TYR:HE1	1:K:93:VAL:HA	1.59	0.68
4:D:163:GLU:HB3	4:D:168:LEU:HD21	1.75	0.68
5:E:247:VAL:HA	5:E:250:THR:HG22	1.74	0.68
2:Q:41:PHE:CE2	2:Q:98:VAL:HG22	2.29	0.68
1:Z:31:ARG:HD3	2:1:127:GLN:OE1	1.93	0.68
2:G:41:PHE:CE2	2:G:98:VAL:HG22	2.29	0.68
5:T:59:SER:HB2	5:T:164:LYS:HG3	1.75	0.68
5:O:247:VAL:HA	5:O:250:THR:HG22	1.75	0.67
5:J:147:ASP:OD2	5:J:151:LYS:NZ	2.18	0.67
1:A:42:TYR:HE1	1:A:93:VAL:HA	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:247:VAL:HA	5:J:250:THR:HG22	1.77	0.67
5:Y:54:GLN:HE21	5:Y:205:THR:HG23	1.59	0.67
8:4:1002:NAG:O7	8:4:1002:NAG:O3	2.13	0.67
5:4:115:ASP:HB3	5:4:118:ALA:HB3	1.75	0.67
5:E:115:ASP:HB3	5:E:118:ALA:HB3	1.75	0.67
5:J:59:SER:HB2	5:J:164:LYS:HG3	1.76	0.67
5:Y:247:VAL:HA	5:Y:250:THR:HG22	1.76	0.67
3:W:193:LEU:HD13	3:W:219:LEU:HD21	1.77	0.67
5:O:115:ASP:HB3	5:O:118:ALA:HB3	1.75	0.67
3:W:261:ILE:HD13	3:W:367:ALA:HB2	1.77	0.67
5:Y:68:THR:HG21	5:Y:248:ARG:HH21	1.60	0.67
3:C:196:THR:OG1	3:C:199:ASN:OD1	2.10	0.67
3:2:267:ASP:HB2	3:2:389:THR:HG21	1.77	0.67
5:4:68:THR:HG21	5:4:248:ARG:HH21	1.61	0.66
3:C:267:ASP:HB2	3:C:389:THR:HG21	1.76	0.66
5:T:115:ASP:HB3	5:T:118:ALA:HB3	1.76	0.66
5:J:54:GLN:HE21	5:J:205:THR:HG23	1.60	0.66
5:Y:59:SER:HB2	5:Y:164:LYS:HG3	1.76	0.66
4:D:86:ALA:N	4:D:88:GLU:OE2	2.28	0.66
3:H:261:ILE:HD13	3:H:367:ALA:HB2	1.78	0.66
5:Y:115:ASP:HB3	5:Y:118:ALA:HB3	1.77	0.66
5:E:43:ASP:CG	5:E:47:LYS:HE2	2.14	0.66
3:M:267:ASP:HB2	3:M:389:THR:HG21	1.76	0.66
3:M:109:TYR:OH	3:R:96:PRO:O	2.09	0.66
3:2:193:LEU:HD13	3:2:219:LEU:HD21	1.77	0.66
3:R:261:ILE:HD13	3:R:367:ALA:HB2	1.78	0.66
5:Y:166:LYS:HB3	5:Y:233:VAL:HG12	1.78	0.66
5:4:117:LYS:NZ	5:4:284:GLU:OE1	2.28	0.65
4:I:86:ALA:N	4:I:88:GLU:OE2	2.30	0.65
4:3:163:GLU:HB3	4:3:168:LEU:HD21	1.78	0.65
4:X:173:VAL:HG11	4:X:186:ARG:HD2	1.78	0.65
3:H:193:LEU:HD13	3:H:219:LEU:HD21	1.77	0.65
3:H:267:ASP:HB2	3:H:389:THR:HG21	1.79	0.65
5:J:39:LEU:H	5:J:223:LEU:HD11	1.61	0.65
5:T:39:LEU:H	5:T:223:LEU:HD11	1.61	0.65
3:C:345:ASP:CG	3:C:346:THR:H	2.00	0.65
4:X:163:GLU:HB3	4:X:168:LEU:HD21	1.78	0.65
5:J:115:ASP:HB3	5:J:118:ALA:HB3	1.77	0.65
2:V:41:PHE:CE2	2:V:98:VAL:HG22	2.32	0.65
3:R:345:ASP:CG	3:R:346:THR:H	1.99	0.65
3:M:351:ALA:HA	3:M:371:LEU:HB3	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:147:ASP:OD2	5:O:151:LYS:NZ	2.21	0.65
5:E:39:LEU:H	5:E:223:LEU:HD11	1.62	0.65
3:R:351:ALA:HA	3:R:371:LEU:HB3	1.77	0.64
3:W:128:ASN:HB3	3:W:130:GLU:H	1.61	0.64
3:M:223:LYS:HD3	3:M:257:ARG:HH11	1.60	0.64
4:S:163:GLU:HB3	4:S:168:LEU:HD21	1.79	0.64
3:W:267:ASP:HB2	3:W:389:THR:HG21	1.77	0.64
1:P:31:ARG:HD3	2:Q:127:GLN:OE1	1.98	0.64
3:R:267:ASP:HB2	3:R:389:THR:HG21	1.80	0.64
5:T:166:LYS:HB3	5:T:233:VAL:HG12	1.79	0.64
5:4:54:GLN:HE21	5:4:205:THR:HG23	1.63	0.64
3:H:196:THR:OG1	3:H:199:ASN:OD1	2.10	0.64
3:M:264:PRO:HB2	3:M:266:LYS:O	1.98	0.64
4:N:163:GLU:HB3	4:N:168:LEU:HD21	1.79	0.64
5:E:166:LYS:HB3	5:E:233:VAL:HG12	1.80	0.64
3:M:345:ASP:CG	3:M:346:THR:H	2.01	0.64
4:N:86:ALA:N	4:N:88:GLU:OE2	2.30	0.64
6:P:201:HEM:HMB1	6:P:201:HEM:HBB2	1.80	0.64
1:U:42:TYR:HE1	1:U:93:VAL:HA	1.63	0.64
4:I:163:GLU:HB3	4:I:168:LEU:HD21	1.80	0.64
1:U:31:ARG:HD3	2:V:127:GLN:OE1	1.97	0.64
5:4:39:LEU:H	5:4:223:LEU:HD11	1.62	0.64
4:X:86:ALA:N	4:X:88:GLU:OE2	2.30	0.64
2:1:41:PHE:CE2	2:1:98:VAL:HG22	2.33	0.64
1:K:31:ARG:HD3	2:L:127:GLN:OE1	1.97	0.64
3:C:223:LYS:HD3	3:C:257:ARG:HH11	1.61	0.64
5:J:68:THR:HG21	5:J:248:ARG:HH21	1.62	0.64
3:M:174:LYS:HB2	3:M:280:TRP:CD1	2.33	0.64
3:R:128:ASN:HB3	3:R:130:GLU:H	1.63	0.63
5:E:147:ASP:OD2	5:E:151:LYS:NZ	2.21	0.63
3:M:128:ASN:HB3	3:M:130:GLU:H	1.62	0.63
5:Y:39:LEU:H	5:Y:223:LEU:HD11	1.63	0.63
3:W:351:ALA:HA	3:W:371:LEU:HB3	1.79	0.63
1:Z:42:TYR:HE1	1:Z:93:VAL:HA	1.63	0.63
4:3:86:ALA:N	4:3:88:GLU:OE2	2.32	0.63
3:H:128:ASN:HB3	3:H:130:GLU:H	1.64	0.63
4:S:173:VAL:HG11	4:S:186:ARG:HD2	1.80	0.63
1:F:42:TYR:HE1	1:F:93:VAL:HA	1.63	0.63
5:O:117:LYS:NZ	5:O:284:GLU:OE1	2.29	0.63
4:D:173:VAL:HG11	4:D:186:ARG:HD2	1.81	0.63
3:H:223:LYS:HD3	3:H:257:ARG:HH11	1.61	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:25:GLY:HA2	2:L:64:GLY:HA3	1.81	0.63
3:M:119:THR:HG23	3:M:121:GLY:HA3	1.81	0.63
5:T:54:GLN:HE21	5:T:205:THR:HG23	1.64	0.63
3:2:261:ILE:HD13	3:2:367:ALA:HB2	1.80	0.63
2:G:95:LYS:HE3	5:J:201:SER:O	1.98	0.62
3:2:128:ASN:HB3	3:2:130:GLU:H	1.64	0.62
5:J:117:LYS:NZ	5:J:284:GLU:OE1	2.30	0.62
3:M:142:LEU:HD11	3:R:96:PRO:HG2	1.80	0.62
1:K:42:TYR:CE1	1:K:93:VAL:HA	2.33	0.62
5:O:166:LYS:HB3	5:O:233:VAL:HG12	1.82	0.62
1:A:98:PHE:HB3	1:A:133:SER:OG	1.99	0.62
1:A:31:ARG:HD3	2:B:127:GLN:OE1	1.99	0.62
5:E:117:LYS:NZ	5:E:284:GLU:OE1	2.30	0.62
6:1:201:HEM:HHD	6:1:201:HEM:HBC2	1.82	0.62
5:T:117:LYS:NZ	5:T:284:GLU:OE1	2.31	0.62
5:E:46:GLU:O	5:E:49:CYS:N	2.32	0.62
1:A:42:TYR:CE1	1:A:93:VAL:HA	2.34	0.62
5:T:68:THR:HG21	5:T:248:ARG:HH21	1.64	0.62
3:2:351:ALA:HA	3:2:371:LEU:HB3	1.80	0.62
3:2:223:LYS:HD3	3:2:257:ARG:HH11	1.63	0.62
6:L:201:HEM:HBC2	6:L:201:HEM:HHD	1.81	0.62
4:N:173:VAL:HG11	4:N:186:ARG:HD2	1.82	0.62
5:O:39:LEU:H	5:O:223:LEU:HD11	1.64	0.62
5:E:126:THR:O	5:E:130:GLU:HG2	2.00	0.61
3:H:351:ALA:HA	3:H:371:LEU:HB3	1.81	0.61
5:O:68:THR:HG21	5:O:248:ARG:HH21	1.65	0.61
2:V:95:LYS:HE3	5:Y:201:SER:O	1.99	0.61
3:W:223:LYS:HD3	3:W:257:ARG:HH11	1.63	0.61
2:1:25:GLY:HA2	2:1:64:GLY:HA3	1.82	0.61
5:J:39:LEU:N	5:J:223:LEU:HD21	2.15	0.61
3:2:196:THR:OG1	3:2:199:ASN:OD1	2.14	0.61
3:W:196:THR:OG1	3:W:199:ASN:OD1	2.14	0.61
3:W:142:LEU:HD11	3:2:96:PRO:HG2	1.82	0.61
1:F:31:ARG:HD3	2:G:127:GLN:OE1	2.01	0.61
2:B:25:GLY:HA2	2:B:64:GLY:HA3	1.83	0.61
2:L:19:ASN:ND2	2:L:22:GLU:HB2	2.16	0.61
3:C:264:PRO:HB2	3:C:266:LYS:O	2.01	0.61
1:F:84:SER:HB3	1:F:139:LYS:HD2	1.82	0.61
3:R:223:LYS:HD3	3:R:257:ARG:HH11	1.64	0.61
3:H:345:ASP:CG	3:H:346:THR:H	2.03	0.61
3:M:332:GLU:OE2	8:M:1005:NAG:H62	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:117:LYS:NZ	5:Y:284:GLU:OE1	2.30	0.61
5:E:68:THR:HG21	5:E:248:ARG:HH21	1.66	0.61
4:3:173:VAL:HG11	4:3:186:ARG:HD2	1.82	0.60
3:C:130:GLU:OE1	3:C:130:GLU:N	2.34	0.60
1:K:17:VAL:HG13	1:K:24:TYR:CE1	2.35	0.60
3:C:119:THR:HG23	3:C:121:GLY:HA3	1.83	0.60
2:G:25:GLY:HA2	2:G:64:GLY:HA3	1.83	0.60
3:C:145:CYS:HB2	3:H:99:ALA:O	2.01	0.60
5:E:110:LEU:HD21	5:E:288:ALA:HB1	1.83	0.60
1:U:42:TYR:CE1	1:U:93:VAL:HA	2.36	0.60
3:2:345:ASP:CG	3:2:346:THR:H	2.03	0.60
1:F:98:PHE:HB3	1:F:133:SER:OG	2.02	0.60
3:M:336:CYS:SG	3:M:384:VAL:HG23	2.42	0.60
5:Y:110:LEU:HD21	5:Y:288:ALA:HB1	1.83	0.60
2:L:95:LYS:HE3	5:O:201:SER:O	2.02	0.60
5:4:39:LEU:N	5:4:223:LEU:HD21	2.16	0.60
1:F:42:TYR:CE1	1:F:93:VAL:HA	2.36	0.60
1:P:42:TYR:HE1	1:P:93:VAL:HA	1.66	0.60
5:T:39:LEU:N	5:T:223:LEU:HD21	2.16	0.60
2:Q:25:GLY:HA2	2:Q:64:GLY:HA3	1.83	0.60
2:Q:41:PHE:HE2	2:Q:98:VAL:HG22	1.66	0.60
3:M:145:CYS:HB2	3:R:99:ALA:O	2.01	0.60
3:W:345:ASP:CG	3:W:346:THR:H	2.05	0.60
3:C:373:PHE:CB	3:C:384:VAL:HG12	2.32	0.60
4:I:173:VAL:HG11	4:I:186:ARG:HD2	1.83	0.60
5:J:110:LEU:HD21	5:J:288:ALA:HB1	1.83	0.60
5:Y:39:LEU:N	5:Y:223:LEU:HD21	2.17	0.60
1:Z:42:TYR:CE1	1:Z:93:VAL:HA	2.36	0.60
3:2:174:LYS:HB2	3:2:280:TRP:CD1	2.37	0.59
3:C:128:ASN:HB3	3:C:130:GLU:H	1.66	0.59
1:Z:17:VAL:HG13	1:Z:24:TYR:CE1	2.36	0.59
5:4:110:LEU:HD21	5:4:288:ALA:HB1	1.83	0.59
3:C:142:LEU:HD11	3:H:96:PRO:HG2	1.83	0.59
2:L:106:LEU:HD23	6:L:201:HEM:CBB	2.31	0.59
2:V:41:PHE:HE2	2:V:98:VAL:HG22	1.66	0.59
5:O:39:LEU:N	5:O:223:LEU:HD21	2.17	0.59
3:R:219:LEU:HD12	3:R:220:TYR:H	1.68	0.59
5:T:110:LEU:HD21	5:T:288:ALA:HB1	1.83	0.59
2:V:25:GLY:HA2	2:V:64:GLY:HA3	1.84	0.59
5:O:110:LEU:HD21	5:O:288:ALA:HB1	1.83	0.59
2:1:95:LYS:HE3	5:4:201:SER:O	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:151:LYS:H	3:M:259:MET:CE	2.16	0.59
2:Q:95:LYS:HE3	5:T:201:SER:O	2.01	0.59
1:U:58:HIS:NE2	7:U:202:OXY:O1	2.36	0.59
5:E:39:LEU:N	5:E:223:LEU:HD21	2.18	0.59
3:H:350:ASP:O	3:H:371:LEU:HD12	2.03	0.59
3:W:174:LYS:HB2	3:W:280:TRP:CD1	2.38	0.59
3:C:186:THR:HG21	3:C:354:ALA:HB2	1.84	0.58
5:J:38:GLY:HA2	5:J:223:LEU:HG	1.85	0.58
3:R:174:LYS:HB2	3:R:280:TRP:CD1	2.37	0.58
3:H:335:PHE:HD2	3:H:387:LYS:HG2	1.67	0.58
5:J:221:GLY:C	5:J:223:LEU:H	2.05	0.58
1:K:84:SER:HB3	1:K:139:LYS:HD2	1.86	0.58
2:B:19:ASN:ND2	2:B:22:GLU:HB2	2.19	0.58
1:A:17:VAL:HG13	1:A:24:TYR:CE1	2.37	0.58
2:G:41:PHE:HE2	2:G:98:VAL:HG22	1.67	0.58
2:L:97:HIS:HB3	3:M:163:LEU:HD12	1.85	0.58
1:P:42:TYR:CE1	1:P:93:VAL:HA	2.38	0.58
5:E:36:ALA:N	3:R:238:TYR:HH	2.02	0.58
1:K:98:PHE:HB3	1:K:133:SER:OG	2.03	0.58
8:C:1006:NAG:O3	8:C:1006:NAG:O7	2.19	0.58
2:B:97:HIS:HB3	3:C:163:LEU:HD12	1.85	0.58
3:R:335:PHE:HD2	3:R:387:LYS:HG2	1.67	0.58
3:W:186:THR:HG21	3:W:354:ALA:HB2	1.85	0.58
5:O:282:ILE:HG12	5:O:285:VAL:HG11	1.86	0.58
5:T:221:GLY:C	5:T:223:LEU:H	2.06	0.58
5:T:38:GLY:HA2	5:T:223:LEU:HG	1.85	0.58
3:2:219:LEU:HD12	3:2:220:TYR:H	1.69	0.57
5:E:282:ILE:HG12	5:E:285:VAL:HG11	1.86	0.57
5:Y:221:GLY:C	5:Y:223:LEU:H	2.06	0.57
5:E:43:ASP:O	5:E:46:GLU:CG	2.53	0.57
5:Y:146:ARG:O	5:Y:149:VAL:HG12	2.04	0.57
3:C:371:LEU:HD13	3:C:385:TYR:CE2	2.39	0.57
5:E:76:VAL:HG21	5:E:146:ARG:HA	1.86	0.57
3:M:186:THR:HG21	3:M:354:ALA:HB2	1.86	0.57
5:O:56:LYS:NZ	5:O:59:SER:OG	2.37	0.57
6:Q:201:HEM:HBC2	6:Q:201:HEM:HHH	1.86	0.57
1:U:17:VAL:HG13	1:U:24:TYR:CE1	2.38	0.57
3:W:179:HIS:HB3	8:W:1002:NAG:H83	1.86	0.57
5:Y:107:LEU:HD22	5:Y:111:GLY:HA3	1.86	0.57
1:F:17:VAL:HG13	1:F:24:TYR:CE1	2.38	0.57
8:H:1004:NAG:O7	8:H:1004:NAG:O3	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:107:LEU:HD22	5:J:111:GLY:HA3	1.86	0.57
3:C:174:LYS:HB2	3:C:280:TRP:CD1	2.39	0.57
3:H:119:THR:HG23	3:H:121:GLY:HA3	1.85	0.57
3:H:255:ASN:OD1	3:H:257:ARG:HG2	2.05	0.57
3:M:219:LEU:HD12	3:M:220:TYR:H	1.69	0.57
1:P:84:SER:HB3	1:P:139:LYS:HD2	1.85	0.57
5:T:107:LEU:HD22	5:T:111:GLY:HA3	1.87	0.57
2:G:19:ASN:ND2	2:G:22:GLU:HB2	2.20	0.57
3:H:174:LYS:HB2	3:H:280:TRP:CD1	2.39	0.57
5:O:107:LEU:HD22	5:O:111:GLY:HA3	1.87	0.57
2:Q:19:ASN:ND2	2:Q:22:GLU:HB2	2.20	0.57
1:Z:11:LYS:NZ	4:3:151:ASN:OD1	2.38	0.57
1:Z:58:HIS:NE2	7:Z:202:OXY:O1	2.38	0.57
5:4:51:LEU:HD21	5:4:214:ILE:HD13	1.86	0.57
3:H:151:LYS:H	3:H:259:MET:CE	2.18	0.57
1:P:98:PHE:HB3	1:P:133:SER:OG	2.05	0.57
3:R:350:ASP:O	3:R:371:LEU:HD12	2.05	0.57
1:U:3:SER:N	1:U:6:ASP:OD2	2.36	0.57
5:Y:282:ILE:HG12	5:Y:285:VAL:HG11	1.86	0.57
8:T:1002:NAG:O7	8:T:1002:NAG:O3	2.16	0.57
3:W:219:LEU:HD12	3:W:220:TYR:H	1.68	0.57
5:4:38:GLY:HA2	5:4:223:LEU:HG	1.86	0.57
5:E:107:LEU:HD22	5:E:111:GLY:HA3	1.87	0.57
5:O:76:VAL:HG21	5:O:146:ARG:HA	1.86	0.57
3:R:373:PHE:CB	3:R:384:VAL:HG12	2.33	0.57
5:T:206:SER:HB3	5:T:208:THR:H	1.70	0.57
2:1:41:PHE:HE2	2:1:98:VAL:HG22	1.70	0.56
5:4:221:GLY:C	5:4:223:LEU:H	2.07	0.56
6:L:201:HEM:HHA	6:L:201:HEM:HBA2	1.87	0.56
3:R:221:VAL:HG23	3:R:225:GLN:HB3	1.86	0.56
6:1:201:HEM:HBA2	6:1:201:HEM:HHA	1.87	0.56
3:C:219:LEU:HD12	3:C:220:TYR:H	1.70	0.56
3:C:335:PHE:HD2	3:C:387:LYS:HG2	1.69	0.56
5:E:206:SER:HB3	5:E:208:THR:H	1.69	0.56
3:2:183:THR:HB	3:2:199:ASN:ND2	2.16	0.56
3:M:335:PHE:HD2	3:M:387:LYS:HG2	1.70	0.56
5:O:221:GLY:C	5:O:223:LEU:H	2.07	0.56
2:Q:122:PHE:CE2	2:Q:127:GLN:HB2	2.40	0.56
3:W:335:PHE:HD2	3:W:387:LYS:HG2	1.70	0.56
3:2:373:PHE:CB	3:2:384:VAL:HG12	2.34	0.56
3:H:219:LEU:HD12	3:H:220:TYR:H	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:350:ASP:O	3:M:371:LEU:HD12	2.06	0.56
5:T:146:ARG:O	5:T:149:VAL:HG12	2.05	0.56
5:E:221:GLY:C	5:E:223:LEU:H	2.08	0.56
6:G:201:HEM:HHD	6:G:201:HEM:HBC2	1.88	0.56
1:P:44:PRO:HB2	1:P:45:HIS:ND1	2.20	0.56
3:R:230:GLU:HB2	3:R:249:LYS:HA	1.87	0.56
2:V:97:HIS:HB3	3:W:163:LEU:HD12	1.87	0.56
5:Y:76:VAL:HG21	5:Y:146:ARG:HA	1.87	0.56
1:F:44:PRO:HB2	1:F:45:HIS:ND1	2.20	0.56
1:K:44:PRO:HB2	1:K:45:HIS:ND1	2.20	0.56
1:P:17:VAL:HG13	1:P:24:TYR:CE1	2.40	0.56
3:R:255:ASN:OD1	3:R:257:ARG:HG2	2.06	0.56
2:1:19:ASN:ND2	2:1:22:GLU:HB2	2.21	0.56
5:J:76:VAL:HG21	5:J:146:ARG:HA	1.87	0.56
8:M:1006:NAG:O3	8:M:1006:NAG:O7	2.22	0.56
3:M:221:VAL:HG23	3:M:225:GLN:HB3	1.86	0.56
5:O:146:ARG:O	5:O:149:VAL:HG12	2.04	0.56
3:R:186:THR:HG21	3:R:354:ALA:HB2	1.88	0.56
5:Y:38:GLY:HA2	5:Y:223:LEU:HG	1.87	0.56
5:4:146:ARG:O	5:4:149:VAL:HG12	2.05	0.56
5:J:282:ILE:HG12	5:J:285:VAL:HG11	1.86	0.56
5:O:38:GLY:HA2	5:O:223:LEU:HG	1.85	0.56
5:O:65:ILE:HG22	5:O:244:VAL:HG21	1.87	0.56
5:4:282:ILE:HG12	5:4:285:VAL:HG11	1.87	0.56
1:A:44:PRO:HB2	1:A:45:HIS:ND1	2.20	0.56
5:T:282:ILE:HG12	5:T:285:VAL:HG11	1.86	0.56
1:Z:98:PHE:HB3	1:Z:133:SER:OG	2.06	0.56
5:4:107:LEU:HD22	5:4:111:GLY:HA3	1.88	0.56
5:J:108:LYS:HA	5:J:112:LYS:HG2	1.88	0.56
3:M:130:GLU:N	3:M:130:GLU:OE1	2.39	0.56
3:M:186:THR:HG23	3:M:352:GLY:O	2.06	0.55
5:T:51:LEU:HD21	5:T:214:ILE:HD13	1.88	0.55
5:T:108:LYS:HA	5:T:112:LYS:HG2	1.88	0.55
3:2:151:LYS:H	3:2:259:MET:CE	2.19	0.55
2:V:63:HIS:NE2	7:V:202:OXY:O1	2.40	0.55
3:W:119:THR:HG23	3:W:121:GLY:HA3	1.88	0.55
3:W:264:PRO:HB2	3:W:266:LYS:O	2.07	0.55
2:1:97:HIS:HB3	3:2:163:LEU:HD12	1.88	0.55
1:A:92:ARG:NH1	1:A:141:ARG:O	2.38	0.55
3:R:128:ASN:HB3	3:R:130:GLU:N	2.21	0.55
5:T:76:VAL:HG21	5:T:146:ARG:HA	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:119:THR:HG23	3:2:121:GLY:HA3	1.87	0.55
3:C:151:LYS:H	3:C:259:MET:CE	2.19	0.55
5:J:206:SER:HB3	5:J:208:THR:H	1.72	0.55
5:O:126:THR:O	5:O:130:GLU:HG2	2.07	0.55
5:Y:51:LEU:HD21	5:Y:214:ILE:HD13	1.88	0.55
1:K:92:ARG:NH1	1:K:141:ARG:O	2.39	0.55
5:4:206:SER:HB3	5:4:208:THR:H	1.72	0.55
2:B:95:LYS:HE3	5:E:201:SER:O	2.07	0.55
5:T:173:ASP:O	5:T:176:VAL:HG12	2.06	0.55
5:Y:173:ASP:O	5:Y:176:VAL:HG12	2.06	0.55
3:H:128:ASN:HB3	3:H:130:GLU:N	2.22	0.55
5:J:146:ARG:O	5:J:149:VAL:HG12	2.06	0.55
3:R:120:GLU:N	3:R:121:GLY:HA3	2.21	0.55
1:F:3:SER:N	1:F:6:ASP:OD2	2.35	0.55
3:H:373:PHE:CB	3:H:384:VAL:HG12	2.36	0.55
1:U:92:ARG:NH1	1:U:141:ARG:O	2.39	0.55
3:2:130:GLU:OE1	3:2:130:GLU:N	2.40	0.55
2:B:106:LEU:HD23	6:B:201:HEM:CBB	2.37	0.55
3:H:230:GLU:HB2	3:H:249:LYS:HA	1.89	0.55
5:4:76:VAL:HG21	5:4:146:ARG:HA	1.89	0.54
5:E:38:GLY:HA2	5:E:223:LEU:HG	1.87	0.54
3:H:186:THR:HG21	3:H:354:ALA:HB2	1.89	0.54
1:A:6:ASP:O	1:A:10:VAL:HG23	2.07	0.54
2:B:106:LEU:HD23	6:B:201:HEM:HBB2	1.88	0.54
3:C:371:LEU:HD13	3:C:385:TYR:CZ	2.43	0.54
5:J:221:GLY:C	5:J:223:LEU:N	2.61	0.54
5:O:51:LEU:HD21	5:O:214:ILE:HD13	1.88	0.54
3:R:119:THR:HG23	3:R:121:GLY:HA3	1.88	0.54
5:Y:47:LYS:HD3	5:Y:216:ALA:O	2.08	0.54
4:D:158:LYS:O	4:D:200:SER:HA	2.07	0.54
3:H:130:GLU:N	3:H:130:GLU:OE1	2.40	0.54
3:M:254:VAL:HG13	3:M:259:MET:HB2	1.88	0.54
5:O:47:LYS:HD3	5:O:216:ALA:O	2.08	0.54
5:Y:126:THR:O	5:Y:130:GLU:HG2	2.08	0.54
3:C:230:GLU:HB2	3:C:249:LYS:HA	1.89	0.54
3:M:230:GLU:HB2	3:M:249:LYS:HA	1.89	0.54
3:R:186:THR:HG23	3:R:352:GLY:O	2.07	0.54
5:T:221:GLY:C	5:T:223:LEU:N	2.61	0.54
5:T:65:ILE:HG22	5:T:244:VAL:HG21	1.89	0.54
2:V:122:PHE:CE2	2:V:127:GLN:HB2	2.42	0.54
5:Y:108:LYS:HA	5:Y:112:LYS:HG2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:84:SER:HB3	1:Z:139:LYS:HD2	1.88	0.54
3:2:332:GLU:OE2	8:2:1004:NAG:H62	2.08	0.54
3:C:184:GLY:O	3:C:352:GLY:HA3	2.08	0.54
3:H:254:VAL:HG13	3:H:259:MET:HB2	1.89	0.54
3:2:230:GLU:HB2	3:2:249:LYS:HA	1.89	0.54
4:3:194:GLN:HG3	4:3:222:PRO:HA	1.90	0.54
1:F:129:LEU:O	1:F:133:SER:HB2	2.08	0.54
3:H:264:PRO:HB2	3:H:266:LYS:O	2.07	0.54
3:M:337:ALA:HB3	3:M:385:TYR:HE1	1.73	0.54
5:O:226:HIS:O	5:O:229:LYS:HG2	2.08	0.54
3:W:230:GLU:HB2	3:W:249:LYS:HA	1.90	0.54
5:E:146:ARG:O	5:E:149:VAL:HG12	2.07	0.54
5:J:191:LYS:NZ	5:J:195:GLU:OE2	2.40	0.54
3:M:373:PHE:CB	3:M:384:VAL:HG12	2.32	0.54
3:R:130:GLU:OE1	3:R:130:GLU:N	2.41	0.54
5:E:173:ASP:O	5:E:176:VAL:HG12	2.07	0.54
5:E:56:LYS:NZ	5:E:59:SER:OG	2.41	0.54
3:M:162:HIS:HB3	3:M:294:TYR:CE2	2.42	0.54
3:M:188:ILE:HG12	3:M:263:LEU:HD11	1.90	0.54
5:T:126:THR:O	5:T:130:GLU:HG2	2.08	0.54
3:2:335:PHE:HD2	3:2:387:LYS:HG2	1.72	0.54
5:4:173:ASP:O	5:4:176:VAL:HG12	2.07	0.54
1:A:84:SER:HB3	1:A:139:LYS:HD2	1.90	0.54
3:C:254:VAL:HG13	3:C:259:MET:HB2	1.88	0.54
5:J:226:HIS:O	5:J:229:LYS:HG2	2.07	0.54
5:J:51:LEU:HD21	5:J:214:ILE:HD13	1.90	0.54
3:M:128:ASN:HB3	3:M:130:GLU:N	2.22	0.54
3:M:142:LEU:HD11	3:R:96:PRO:CG	2.38	0.54
5:O:173:ASP:O	5:O:176:VAL:HG12	2.07	0.54
5:Y:221:GLY:C	5:Y:223:LEU:N	2.61	0.54
3:2:186:THR:HG21	3:2:354:ALA:HB2	1.90	0.54
3:C:186:THR:HG23	3:C:352:GLY:O	2.08	0.54
3:H:221:VAL:HG23	3:H:225:GLN:HB3	1.89	0.54
3:W:151:LYS:H	3:W:259:MET:CE	2.20	0.54
1:F:92:ARG:NH1	1:F:141:ARG:O	2.40	0.53
2:G:122:PHE:CE2	2:G:127:GLN:HB2	2.43	0.53
3:H:151:LYS:H	3:H:259:MET:HE1	1.73	0.53
3:H:271:VAL:HA	3:H:299:VAL:HG22	1.89	0.53
5:J:173:ASP:O	5:J:176:VAL:HG12	2.07	0.53
5:J:47:LYS:HD3	5:J:216:ALA:O	2.08	0.53
3:2:128:ASN:HB3	3:2:130:GLU:N	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:255:ASN:OD1	3:2:257:ARG:HG2	2.09	0.53
5:E:65:ILE:HG22	5:E:244:VAL:HG21	1.91	0.53
1:P:92:ARG:NH1	1:P:141:ARG:O	2.41	0.53
5:T:47:LYS:HD3	5:T:216:ALA:O	2.07	0.53
3:2:221:VAL:HG23	3:2:225:GLN:HB3	1.90	0.53
3:2:264:PRO:HB2	3:2:266:LYS:O	2.08	0.53
5:4:65:ILE:HG22	5:4:244:VAL:HG21	1.90	0.53
3:W:254:VAL:HG13	3:W:259:MET:HB2	1.89	0.53
5:4:221:GLY:C	5:4:223:LEU:N	2.61	0.53
5:E:51:LEU:HD21	5:E:214:ILE:HD13	1.90	0.53
3:H:120:GLU:N	3:H:121:GLY:HA3	2.23	0.53
3:W:120:GLU:N	3:W:121:GLY:HA3	2.22	0.53
1:F:83:LEU:HD11	6:F:201:HEM:HMA1	1.90	0.53
3:W:128:ASN:HB3	3:W:130:GLU:N	2.23	0.53
3:W:130:GLU:N	3:W:130:GLU:OE1	2.41	0.53
1:Z:44:PRO:HB2	1:Z:45:HIS:ND1	2.23	0.53
2:B:122:PHE:CE2	2:B:127:GLN:HB2	2.44	0.53
5:J:126:THR:O	5:J:130:GLU:HG2	2.09	0.53
4:S:194:GLN:HG3	4:S:222:PRO:HA	1.91	0.53
4:3:198:ILE:HB	4:3:215:THR:HB	1.91	0.53
5:T:226:HIS:O	5:T:229:LYS:HG2	2.08	0.53
1:Z:3:SER:N	1:Z:6:ASP:OD2	2.38	0.53
5:4:47:LYS:HD3	5:4:216:ALA:O	2.08	0.53
4:N:158:LYS:O	4:N:200:SER:HA	2.09	0.53
5:O:206:SER:HB3	5:O:208:THR:H	1.73	0.53
3:R:151:LYS:H	3:R:259:MET:CE	2.22	0.53
3:W:221:VAL:HG23	3:W:225:GLN:HB3	1.90	0.53
3:2:120:GLU:N	3:2:121:GLY:HA3	2.23	0.53
3:C:162:HIS:HB3	3:C:294:TYR:CE2	2.43	0.53
3:H:332:GLU:OE2	8:H:1003:NAG:H62	2.09	0.53
5:O:221:GLY:C	5:O:223:LEU:N	2.62	0.53
1:P:3:SER:N	1:P:6:ASP:OD2	2.37	0.53
5:4:126:THR:O	5:4:130:GLU:HG2	2.09	0.53
3:M:120:GLU:N	3:M:121:GLY:HA3	2.23	0.53
3:R:254:VAL:HG13	3:R:259:MET:HB2	1.90	0.53
1:Z:92:ARG:NH1	1:Z:141:ARG:O	2.41	0.53
3:H:336:CYS:SG	3:H:384:VAL:HG23	2.49	0.52
5:E:221:GLY:C	5:E:223:LEU:N	2.62	0.52
2:L:122:PHE:CE2	2:L:127:GLN:HB2	2.44	0.52
5:4:43:ASP:OD2	5:4:47:LYS:HE2	2.09	0.52
3:C:332:GLU:OE2	8:C:1005:NAG:H62	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:128:ASN:HB3	3:C:130:GLU:N	2.24	0.52
3:H:186:THR:HG23	3:H:352:GLY:O	2.09	0.52
3:2:254:VAL:HG13	3:2:259:MET:HB2	1.91	0.52
3:R:196:THR:OG1	3:R:199:ASN:OD1	2.19	0.52
1:U:98:PHE:HB3	1:U:133:SER:OG	2.09	0.52
2:V:19:ASN:ND2	2:V:22:GLU:HB2	2.25	0.52
3:2:271:VAL:HA	3:2:299:VAL:HG22	1.91	0.52
1:A:129:LEU:O	1:A:133:SER:HB2	2.10	0.52
5:E:226:HIS:O	5:E:229:LYS:HG2	2.10	0.52
3:H:374:ASP:OD1	3:H:374:ASP:N	2.30	0.52
1:F:11:LYS:NZ	4:I:151:ASN:OD1	2.38	0.52
5:T:191:LYS:NZ	5:T:195:GLU:OE2	2.42	0.52
5:T:38:GLY:HA3	5:T:177:LEU:HG	1.91	0.52
3:C:120:GLU:N	3:C:121:GLY:HA3	2.24	0.52
1:U:44:PRO:HB2	1:U:45:HIS:ND1	2.24	0.52
5:4:166:LYS:HB3	5:4:233:VAL:HG12	1.91	0.52
3:C:188:ILE:HG12	3:C:263:LEU:HD11	1.92	0.52
2:L:24:GLY:N	2:L:68:LEU:HD22	2.22	0.52
4:X:158:LYS:O	4:X:200:SER:HA	2.10	0.52
6:F:201:HEM:HBB2	6:F:201:HEM:HMB1	1.92	0.51
1:F:107:VAL:HG11	2:G:127:GLN:OE1	2.09	0.51
3:H:340:SER:HB3	3:H:344:GLU:H	1.75	0.51
3:H:340:SER:HB3	3:H:344:GLU:N	2.25	0.51
1:K:17:VAL:HG13	1:K:24:TYR:CD1	2.45	0.51
3:R:302:GLN:O	3:R:306:ILE:HG12	2.09	0.51
3:W:373:PHE:CB	3:W:384:VAL:HG12	2.35	0.51
5:Y:43:ASP:OD2	5:Y:47:LYS:HE2	2.10	0.51
2:B:24:GLY:N	2:B:68:LEU:HD22	2.22	0.51
3:M:151:LYS:H	3:M:259:MET:HE2	1.75	0.51
4:S:94:ILE:HD12	4:S:175:TYR:CZ	2.45	0.51
4:D:194:GLN:HG3	4:D:222:PRO:HA	1.91	0.51
3:H:306:ILE:HD13	3:H:330:LEU:HD13	1.90	0.51
5:J:65:ILE:HG22	5:J:244:VAL:HG21	1.93	0.51
4:N:198:ILE:HB	4:N:215:THR:HB	1.92	0.51
5:4:108:LYS:HA	5:4:112:LYS:HG2	1.92	0.51
1:P:6:ASP:O	1:P:10:VAL:HG23	2.10	0.51
3:2:162:HIS:HB3	3:2:294:TYR:CE2	2.45	0.51
5:4:38:GLY:HA3	5:4:177:LEU:HG	1.91	0.51
3:C:96:PRO:HG2	3:H:142:LEU:HD11	1.93	0.51
4:I:198:ILE:HB	4:I:215:THR:HB	1.93	0.51
5:Y:65:ILE:HG22	5:Y:244:VAL:HG21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:306:ILE:HD13	3:2:330:LEU:HD13	1.91	0.51
3:2:340:SER:HB3	3:2:344:GLU:H	1.75	0.51
1:K:129:LEU:O	1:K:133:SER:HB2	2.11	0.51
1:U:84:SER:HB3	1:U:139:LYS:HD2	1.93	0.51
5:Y:38:GLY:HA3	5:Y:177:LEU:HG	1.92	0.51
3:2:151:LYS:H	3:2:259:MET:HE1	1.74	0.51
4:3:158:LYS:O	4:3:200:SER:HA	2.10	0.51
3:R:271:VAL:HA	3:R:299:VAL:HG22	1.92	0.51
3:R:340:SER:HB3	3:R:344:GLU:H	1.75	0.51
5:E:108:LYS:HA	5:E:112:LYS:HG2	1.91	0.51
4:I:194:GLN:HG3	4:I:222:PRO:HA	1.93	0.51
2:L:18:VAL:HG13	2:L:23:VAL:HG21	1.93	0.51
3:M:303:ASP:HB3	3:M:307:ARG:NH2	2.26	0.51
3:R:119:THR:CG2	3:R:143:PRO:HB3	2.41	0.51
3:R:345:ASP:OD1	3:R:346:THR:HG22	2.11	0.51
4:X:194:GLN:HG3	4:X:222:PRO:HA	1.91	0.51
5:4:191:LYS:NZ	5:4:195:GLU:OE2	2.44	0.51
5:4:226:HIS:O	5:4:229:LYS:HG2	2.10	0.51
1:K:11:LYS:NZ	4:N:151:ASN:OD1	2.43	0.51
5:T:97:LEU:HD21	5:T:129:ARG:HE	1.76	0.51
4:D:113:ASN:ND2	5:O:202:SER:OG	2.44	0.51
5:O:42:LYS:HG3	5:O:193:ALA:HB2	1.93	0.51
3:R:340:SER:HB3	3:R:344:GLU:N	2.26	0.51
3:W:145:CYS:HB2	3:2:99:ALA:O	2.11	0.50
3:C:221:VAL:HG23	3:C:225:GLN:HB3	1.91	0.50
5:E:42:LYS:HG3	5:E:193:ALA:HB2	1.93	0.50
3:C:142:LEU:HD11	3:H:96:PRO:CG	2.42	0.50
5:J:38:GLY:HA3	5:J:177:LEU:HG	1.92	0.50
3:M:271:VAL:HA	3:M:299:VAL:HG22	1.93	0.50
5:O:108:LYS:HA	5:O:112:LYS:HG2	1.92	0.50
5:T:49:CYS:HA	5:T:178:LEU:HD21	1.93	0.50
3:2:162:HIS:HB2	3:2:294:TYR:O	2.10	0.50
5:4:49:CYS:HA	5:4:178:LEU:HD21	1.93	0.50
1:F:35:SER:HB3	2:G:131:GLN:HG3	1.94	0.50
5:O:43:ASP:OD2	5:O:47:LYS:HE2	2.12	0.50
4:S:158:LYS:O	4:S:200:SER:HA	2.11	0.50
2:1:24:GLY:N	2:1:68:LEU:HD22	2.22	0.50
3:C:119:THR:CG2	3:C:143:PRO:HB3	2.41	0.50
3:M:321:LYS:O	3:M:323:PRO:HD3	2.10	0.50
3:M:306:ILE:HD13	3:M:330:LEU:HD13	1.92	0.50
1:U:129:LEU:O	1:U:133:SER:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:302:GLN:O	3:W:306:ILE:HG12	2.11	0.50
2:1:122:PHE:CE2	2:1:127:GLN:HB2	2.46	0.50
2:G:97:HIS:HB3	3:H:163:LEU:HD12	1.93	0.50
3:M:255:ASN:OD1	3:M:257:ARG:HG2	2.11	0.50
4:N:194:GLN:HG3	4:N:222:PRO:HA	1.92	0.50
5:O:191:LYS:NZ	5:O:195:GLU:OE2	2.44	0.50
2:1:106:LEU:HD23	6:1:201:HEM:CBB	2.42	0.50
4:3:131:ILE:HG21	4:3:148:LEU:HD22	1.93	0.50
2:B:109:VAL:O	2:B:113:VAL:HG23	2.11	0.50
5:E:127:SER:HA	5:E:130:GLU:HG2	1.94	0.50
5:J:166:LYS:HB3	5:J:233:VAL:HG12	1.93	0.50
3:M:340:SER:HB3	3:M:344:GLU:H	1.75	0.50
5:Y:226:HIS:O	5:Y:229:LYS:HG2	2.12	0.50
5:Y:287:ASN:O	5:Y:291:THR:OG1	2.18	0.50
4:D:198:ILE:HB	4:D:215:THR:HB	1.93	0.50
5:Y:206:SER:HB3	5:Y:208:THR:H	1.76	0.50
3:H:188:ILE:HG12	3:H:263:LEU:HD11	1.94	0.50
5:J:43:ASP:OD2	5:J:47:LYS:HE2	2.11	0.50
3:M:223:LYS:HD3	3:M:257:ARG:NH1	2.26	0.50
5:T:43:ASP:OD2	5:T:47:LYS:HE2	2.11	0.50
4:3:87:ASP:HB2	4:3:159:PHE:O	2.12	0.50
1:A:17:VAL:HG13	1:A:24:TYR:CD1	2.46	0.50
2:G:24:GLY:N	2:G:68:LEU:HD22	2.23	0.50
3:R:264:PRO:HB2	3:R:266:LYS:O	2.12	0.50
3:W:186:THR:HG23	3:W:352:GLY:O	2.12	0.50
3:H:223:LYS:HD3	3:H:257:ARG:NH1	2.26	0.50
5:J:97:LEU:HD21	5:J:129:ARG:HE	1.77	0.50
5:O:38:GLY:HA3	5:O:177:LEU:HG	1.93	0.50
4:S:87:ASP:HB2	4:S:159:PHE:O	2.12	0.50
2:V:123:THR:OG1	2:V:125:PRO:HD2	2.12	0.50
5:4:56:LYS:NZ	5:4:59:SER:OG	2.44	0.49
2:B:18:VAL:HG13	2:B:23:VAL:HG21	1.94	0.49
3:C:321:LYS:O	3:C:323:PRO:HD3	2.12	0.49
3:H:119:THR:CG2	3:H:143:PRO:HB3	2.42	0.49
4:I:87:ASP:HB2	4:I:159:PHE:O	2.12	0.49
4:S:198:ILE:HB	4:S:215:THR:HB	1.94	0.49
3:W:162:HIS:HB3	3:W:294:TYR:CE2	2.46	0.49
4:X:198:ILE:HB	4:X:215:THR:HB	1.93	0.49
3:2:350:ASP:O	3:2:371:LEU:HD12	2.12	0.49
3:C:337:ALA:HB3	3:C:385:TYR:HE1	1.76	0.49
2:G:75:LEU:HD21	2:G:133:VAL:HG11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:123:THR:OG1	2:B:125:PRO:HD2	2.13	0.49
3:C:114:TYR:O	3:C:148:VAL:HG23	2.12	0.49
5:E:38:GLY:HA3	5:E:177:LEU:HG	1.94	0.49
2:L:123:THR:OG1	2:L:125:PRO:HD2	2.12	0.49
3:M:340:SER:HB3	3:M:344:GLU:N	2.27	0.49
2:Q:75:LEU:HD21	2:Q:133:VAL:HG11	1.94	0.49
1:Z:129:LEU:O	1:Z:133:SER:HB2	2.12	0.49
3:C:296:MET:CE	5:E:71:ARG:HA	2.42	0.49
4:N:87:ASP:HB2	4:N:159:PHE:O	2.11	0.49
3:R:170:PRO:HB2	3:R:259:MET:HG2	1.94	0.49
3:R:238:TYR:N	3:R:238:TYR:CD1	2.81	0.49
3:R:324:VAL:HG23	3:R:326:VAL:H	1.76	0.49
3:2:324:VAL:HG23	3:2:326:VAL:H	1.77	0.49
5:4:97:LEU:HD21	5:4:129:ARG:HE	1.77	0.49
4:D:94:ILE:HD12	4:D:175:TYR:CZ	2.47	0.49
3:C:109:TYR:OH	3:H:96:PRO:O	2.16	0.49
5:J:49:CYS:HA	5:J:178:LEU:HD21	1.94	0.49
3:M:388:VAL:O	3:M:391:ILE:HG13	2.13	0.49
3:M:196:THR:HG21	3:M:351:ALA:HB1	1.95	0.49
1:P:107:VAL:HG11	2:Q:127:GLN:OE1	2.11	0.49
3:W:306:ILE:HD13	3:W:330:LEU:HD13	1.93	0.49
3:2:119:THR:CG2	3:2:143:PRO:HB3	2.43	0.49
5:J:42:LYS:HG3	5:J:193:ALA:HB2	1.95	0.49
4:S:96:ASP:HB3	4:S:99:LEU:HD22	1.95	0.49
3:W:156:ALA:O	3:W:157:ASN:HB2	2.13	0.49
1:Z:83:LEU:HD11	6:Z:201:HEM:HMA1	1.94	0.49
5:J:44:GLU:CD	5:J:221:GLY:HA3	2.33	0.49
1:Z:6:ASP:O	1:Z:10:VAL:HG23	2.12	0.49
1:Z:17:VAL:HG13	1:Z:24:TYR:CD1	2.47	0.49
3:2:340:SER:HB3	3:2:344:GLU:N	2.28	0.49
5:4:42:LYS:HG3	5:4:193:ALA:HB2	1.95	0.49
3:C:114:TYR:CD2	3:C:255:ASN:HA	2.47	0.49
3:M:170:PRO:HB2	3:M:259:MET:HG2	1.95	0.49
3:W:255:ASN:OD1	3:W:257:ARG:HG2	2.12	0.49
3:W:271:VAL:HA	3:W:299:VAL:HG22	1.94	0.49
3:H:350:ASP:C	3:H:371:LEU:HD12	2.34	0.49
4:I:94:ILE:HD12	4:I:175:TYR:CZ	2.47	0.49
4:N:145:GLU:OE2	4:N:171:ARG:NH2	2.40	0.49
3:C:303:ASP:HB3	3:C:307:ARG:NH2	2.28	0.48
3:H:153:LYS:HB3	3:H:256:GLU:HB2	1.94	0.48
3:M:143:PRO:HG2	3:R:98:ILE:HD13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:119:THR:CG2	3:W:143:PRO:HB3	2.43	0.48
5:Y:97:LEU:HD21	5:Y:129:ARG:HE	1.77	0.48
2:1:75:LEU:HD21	2:1:133:VAL:HG11	1.95	0.48
3:2:156:ALA:O	3:2:157:ASN:HB2	2.13	0.48
4:I:158:LYS:O	4:I:200:SER:HA	2.12	0.48
2:Q:123:THR:OG1	2:Q:125:PRO:HD2	2.13	0.48
1:U:6:ASP:O	1:U:10:VAL:HG23	2.12	0.48
2:V:63:HIS:O	2:V:67:VAL:HG23	2.13	0.48
3:W:350:ASP:O	3:W:371:LEU:HD12	2.13	0.48
4:X:96:ASP:HB3	4:X:99:LEU:HD22	1.96	0.48
3:W:142:LEU:HD11	3:2:96:PRO:CG	2.44	0.48
4:D:87:ASP:HB2	4:D:159:PHE:O	2.12	0.48
2:G:123:THR:OG1	2:G:125:PRO:HD2	2.13	0.48
3:H:162:HIS:HB3	3:H:294:TYR:CE2	2.48	0.48
1:K:66:LEU:O	1:K:70:VAL:HG12	2.14	0.48
1:K:107:VAL:HG11	2:L:127:GLN:OE1	2.13	0.48
3:M:107:VAL:HG11	3:R:95:PRO:HG3	1.95	0.48
3:R:114:TYR:CD2	3:R:255:ASN:HA	2.48	0.48
3:R:188:ILE:HG12	3:R:263:LEU:HD11	1.95	0.48
5:T:44:GLU:CD	5:T:221:GLY:HA3	2.33	0.48
4:3:96:ASP:HB3	4:3:99:LEU:HD22	1.96	0.48
4:D:145:GLU:OE2	4:D:171:ARG:NH2	2.41	0.48
4:I:126:TYR:CE2	4:I:202:THR:HG21	2.48	0.48
3:R:340:SER:OG	3:R:341:LYS:N	2.45	0.48
3:C:196:THR:HG21	3:C:351:ALA:HB1	1.95	0.48
4:D:96:ASP:HB3	4:D:99:LEU:HD22	1.96	0.48
3:H:321:LYS:O	3:H:323:PRO:HD3	2.13	0.48
3:H:324:VAL:HG23	3:H:326:VAL:H	1.78	0.48
5:J:256:LYS:HE3	5:J:260:LYS:HE3	1.96	0.48
3:M:119:THR:CG2	3:M:143:PRO:HB3	2.43	0.48
3:R:374:ASP:OD1	3:R:374:ASP:N	2.35	0.48
4:S:131:ILE:HG21	4:S:148:LEU:HD22	1.95	0.48
5:T:42:LYS:HG3	5:T:193:ALA:HB2	1.96	0.48
3:W:119:THR:HG21	3:W:143:PRO:HB3	1.95	0.48
5:Y:191:LYS:NZ	5:Y:195:GLU:OE2	2.44	0.48
4:3:126:TYR:CE2	4:3:202:THR:HG21	2.48	0.48
5:E:121:ILE:O	5:E:125:ILE:HG12	2.13	0.48
3:H:135:ASN:O	3:H:139:GLY:N	2.43	0.48
4:I:131:ILE:HG21	4:I:148:LEU:HD22	1.94	0.48
3:M:162:HIS:HB2	3:M:294:TYR:O	2.13	0.48
2:V:88:LEU:HD21	6:V:201:HEM:HMA3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:162:HIS:HB2	3:C:294:TYR:O	2.13	0.48
3:C:223:LYS:HD3	3:C:257:ARG:NH1	2.28	0.48
2:G:109:VAL:O	2:G:113:VAL:HG23	2.14	0.48
3:H:302:GLN:O	3:H:306:ILE:HG12	2.12	0.48
3:H:345:ASP:OD1	3:H:346:THR:HG22	2.14	0.48
3:M:238:TYR:N	3:M:238:TYR:CD1	2.82	0.48
5:O:39:LEU:HD23	5:O:40:LYS:H	1.79	0.48
2:Q:88:LEU:O	2:Q:92:HIS:ND1	2.42	0.48
3:W:183:THR:HB	3:W:199:ASN:ND2	2.19	0.48
5:Y:49:CYS:HA	5:Y:178:LEU:HD21	1.94	0.48
4:3:145:GLU:OE2	4:3:171:ARG:NH2	2.41	0.48
3:C:238:TYR:N	3:C:238:TYR:CD1	2.82	0.48
3:C:271:VAL:HA	3:C:299:VAL:HG22	1.96	0.48
4:I:96:ASP:HB3	4:I:99:LEU:HD22	1.96	0.48
5:O:49:CYS:HA	5:O:178:LEU:HD21	1.94	0.48
2:Q:109:VAL:O	2:Q:113:VAL:HG23	2.14	0.48
3:2:186:THR:HG23	3:2:352:GLY:O	2.13	0.48
3:C:198:LYS:NZ	3:C:329:ILE:HD11	2.29	0.48
3:C:336:CYS:SG	3:C:384:VAL:HG23	2.53	0.48
1:F:17:VAL:HG13	1:F:24:TYR:CD1	2.48	0.48
1:K:9:ASN:ND2	1:K:121:VAL:HG22	2.24	0.48
3:R:162:HIS:HB3	3:R:294:TYR:CE2	2.49	0.48
3:R:336:CYS:SG	3:R:384:VAL:HG23	2.54	0.48
5:E:44:GLU:CD	5:E:221:GLY:HA3	2.34	0.48
2:G:31:LEU:HD13	2:G:106:LEU:HB2	1.95	0.48
3:M:183:THR:HB	3:M:199:ASN:ND2	2.17	0.48
3:R:350:ASP:C	3:R:371:LEU:HD12	2.35	0.48
4:D:131:ILE:HG21	4:D:148:LEU:HD22	1.96	0.47
3:M:374:ASP:N	3:M:374:ASP:OD1	2.28	0.47
6:Q:201:HEM:CBC	6:Q:201:HEM:HHD	2.44	0.47
1:U:17:VAL:HG13	1:U:24:TYR:CD1	2.49	0.47
5:Y:44:GLU:CD	5:Y:221:GLY:HA3	2.35	0.47
3:H:238:TYR:CD1	3:H:238:TYR:N	2.83	0.47
5:J:38:GLY:O	5:J:39:LEU:HB2	2.14	0.47
3:M:153:LYS:HB3	3:M:256:GLU:HB2	1.96	0.47
3:M:179:HIS:HB3	8:M:1002:NAG:H83	1.95	0.47
5:O:44:GLU:CD	5:O:221:GLY:HA3	2.35	0.47
3:R:223:LYS:HD3	3:R:257:ARG:NH1	2.28	0.47
1:U:107:VAL:HG11	2:V:127:GLN:OE1	2.14	0.47
5:Y:43:ASP:O	5:Y:46:GLU:HG2	2.14	0.47
3:C:151:LYS:H	3:C:259:MET:HE2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:340:SER:HB3	3:C:344:GLU:H	1.78	0.47
3:C:340:SER:HB3	3:C:344:GLU:N	2.29	0.47
3:M:160:GLY:HA3	3:M:344:GLU:HG2	1.96	0.47
3:R:119:THR:HG21	3:R:143:PRO:HB3	1.96	0.47
3:R:153:LYS:HB3	3:R:256:GLU:HB2	1.96	0.47
3:R:306:ILE:HD13	3:R:330:LEU:HD13	1.94	0.47
3:W:337:ALA:HB3	3:W:385:TYR:HE1	1.78	0.47
5:Y:121:ILE:O	5:Y:125:ILE:HG12	2.14	0.47
5:Y:51:LEU:HA	5:Y:51:LEU:HD23	1.72	0.47
3:2:188:ILE:HG12	3:2:263:LEU:HD11	1.96	0.47
3:M:302:GLN:O	3:M:306:ILE:HG12	2.14	0.47
3:R:151:LYS:H	3:R:259:MET:HE1	1.79	0.47
4:S:126:TYR:CE2	4:S:202:THR:HG21	2.49	0.47
4:X:131:ILE:HG21	4:X:148:LEU:HD22	1.96	0.47
4:X:87:ASP:HB2	4:X:159:PHE:O	2.13	0.47
5:Y:42:LYS:HG3	5:Y:193:ALA:HB2	1.96	0.47
2:1:63:HIS:O	2:1:67:VAL:HG23	2.15	0.47
3:2:238:TYR:N	3:2:238:TYR:CD1	2.83	0.47
3:C:119:THR:HG21	3:C:143:PRO:HB3	1.96	0.47
3:H:170:PRO:HB2	3:H:259:MET:HG2	1.96	0.47
2:L:51:PRO:O	2:L:55:MET:HG2	2.15	0.47
3:W:151:LYS:H	3:W:259:MET:HE2	1.79	0.47
3:2:337:ALA:HB3	3:2:385:TYR:HE1	1.79	0.47
3:C:135:ASN:O	3:C:139:GLY:N	2.43	0.47
1:F:6:ASP:O	1:F:10:VAL:HG23	2.13	0.47
2:L:41:PHE:HB3	6:L:201:HEM:HMD2	1.97	0.47
5:T:43:ASP:O	5:T:46:GLU:HG2	2.15	0.47
3:C:302:GLN:O	3:C:306:ILE:HG12	2.14	0.47
3:C:388:VAL:O	3:C:391:ILE:HG13	2.15	0.47
3:M:198:LYS:NZ	3:M:329:ILE:HD11	2.30	0.47
3:M:174:LYS:HB2	3:M:280:TRP:CG	2.49	0.47
3:W:324:VAL:HG23	3:W:326:VAL:H	1.78	0.47
3:2:119:THR:HG21	3:2:143:PRO:HB3	1.97	0.47
3:C:156:ALA:O	3:C:157:ASN:HB2	2.14	0.47
3:C:170:PRO:HB2	3:C:259:MET:HG2	1.97	0.47
5:E:39:LEU:HD23	5:E:40:LYS:H	1.80	0.47
2:Q:24:GLY:N	2:Q:68:LEU:HD22	2.26	0.47
3:W:175:MET:HB2	3:W:219:LEU:HD13	1.95	0.47
3:2:223:LYS:HD3	3:2:257:ARG:NH1	2.29	0.47
3:2:321:LYS:O	3:2:323:PRO:HD3	2.14	0.47
3:H:92:CYS:O	3:H:92:CYS:SG	2.72	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:6:ASP:O	1:K:10:VAL:HG23	2.15	0.47
3:R:245:LEU:HD23	3:R:245:LEU:HA	1.62	0.47
2:V:109:VAL:O	2:V:113:VAL:HG23	2.15	0.47
3:W:238:TYR:CD1	3:W:238:TYR:N	2.83	0.47
3:W:162:HIS:HB2	3:W:294:TYR:O	2.15	0.47
3:C:153:LYS:HB3	3:C:256:GLU:HB2	1.96	0.47
3:C:296:MET:HE1	5:E:71:ARG:HA	1.97	0.47
3:C:374:ASP:N	3:C:374:ASP:OD1	2.29	0.47
4:D:126:TYR:CE2	4:D:202:THR:HG21	2.50	0.47
3:H:245:LEU:HD23	3:H:245:LEU:HA	1.64	0.47
3:M:224:LYS:HE2	3:M:224:LYS:HB3	1.76	0.47
3:M:188:ILE:CG1	3:M:263:LEU:HD11	2.44	0.47
5:O:121:ILE:O	5:O:125:ILE:HG12	2.14	0.47
3:R:303:ASP:HB3	3:R:307:ARG:NH2	2.29	0.47
3:W:312:SER:HB2	3:W:314:VAL:O	2.15	0.47
3:W:345:ASP:OD1	3:W:346:THR:HG22	2.15	0.47
3:2:374:ASP:N	3:2:374:ASP:OD1	2.37	0.47
1:A:11:LYS:NZ	4:D:151:ASN:OD1	2.47	0.47
1:A:66:LEU:O	1:A:70:VAL:HG12	2.15	0.47
5:E:97:LEU:HD21	5:E:129:ARG:HE	1.79	0.47
3:H:119:THR:HG21	3:H:143:PRO:HB3	1.97	0.47
3:M:184:GLY:O	3:M:352:GLY:HA3	2.15	0.47
3:R:388:VAL:O	3:R:391:ILE:HG13	2.14	0.47
3:W:223:LYS:HD3	3:W:257:ARG:NH1	2.29	0.47
4:X:94:ILE:HD12	4:X:175:TYR:CZ	2.50	0.47
2:1:123:THR:OG1	2:1:125:PRO:HD2	2.15	0.46
2:B:71:PHE:CE2	2:B:137:VAL:HG11	2.50	0.46
2:L:101:GLU:OE1	2:L:101:GLU:HA	2.16	0.46
4:N:126:TYR:CE2	4:N:202:THR:HG21	2.50	0.46
2:Q:63:HIS:O	2:Q:67:VAL:HG23	2.15	0.46
3:R:314:VAL:HA	3:R:315:PRO:HD3	1.80	0.46
5:4:44:GLU:CD	5:4:221:GLY:HA3	2.35	0.46
1:A:3:SER:N	1:A:6:ASP:OD2	2.39	0.46
3:C:224:LYS:HB3	3:C:224:LYS:HE2	1.76	0.46
3:H:388:VAL:O	3:H:391:ILE:HG13	2.15	0.46
1:P:129:LEU:O	1:P:133:SER:HB2	2.15	0.46
3:R:321:LYS:O	3:R:323:PRO:HD3	2.15	0.46
3:W:114:TYR:CD2	3:W:255:ASN:HA	2.50	0.46
1:Z:119:PRO:HG2	2:1:55:MET:HG3	1.97	0.46
5:4:38:GLY:O	5:4:39:LEU:HB2	2.15	0.46
5:J:46:GLU:HA	5:J:49:CYS:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:97:LEU:HD21	5:O:129:ARG:HE	1.79	0.46
5:T:38:GLY:O	5:T:39:LEU:HB2	2.15	0.46
1:Z:48:LEU:HA	1:Z:48:LEU:HD23	1.73	0.46
3:2:153:LYS:HB3	3:2:256:GLU:HB2	1.97	0.46
5:4:121:ILE:O	5:4:125:ILE:HG12	2.14	0.46
5:E:173:ASP:OD2	5:E:229:LYS:NZ	2.48	0.46
3:M:119:THR:HG23	3:M:121:GLY:CA	2.45	0.46
3:M:277:VAL:HG12	3:M:278:SER:O	2.16	0.46
3:M:306:ILE:CD1	3:M:330:LEU:HD13	2.46	0.46
4:N:94:ILE:HD12	4:N:175:TYR:CZ	2.50	0.46
1:P:14:TRP:HE1	1:P:67:THR:HG23	1.80	0.46
5:T:46:GLU:HA	5:T:49:CYS:HB3	1.97	0.46
1:U:27:GLU:OE2	1:U:108:THR:HG23	2.16	0.46
3:2:179:HIS:HB3	8:2:1002:NAG:H83	1.97	0.46
8:4:1002:NAG:C7	8:4:1002:NAG:HO3	2.24	0.46
3:C:376:SER:HB2	3:C:380:ALA:O	2.15	0.46
4:N:140:THR:OG1	4:N:143:LYS:O	2.32	0.46
5:O:166:LYS:HD2	5:O:232:ASP:HB2	1.98	0.46
1:P:17:VAL:HG13	1:P:24:TYR:CD1	2.50	0.46
5:T:121:ILE:O	5:T:125:ILE:HG12	2.14	0.46
3:W:188:ILE:HG12	3:W:263:LEU:HD11	1.97	0.46
3:2:245:LEU:HD23	3:2:245:LEU:HA	1.63	0.46
1:A:14:TRP:HE1	1:A:67:THR:HG23	1.81	0.46
3:H:306:ILE:CD1	3:H:330:LEU:HD13	2.45	0.46
3:M:135:ASN:O	3:M:139:GLY:N	2.44	0.46
2:Q:71:PHE:CE2	2:Q:137:VAL:HG11	2.50	0.46
3:R:196:THR:HG21	3:R:351:ALA:HB1	1.97	0.46
3:W:321:LYS:O	3:W:323:PRO:HD3	2.15	0.46
1:Z:65:ALA:HB2	6:Z:201:HEM:HMA1	1.98	0.46
4:3:94:ILE:HD12	4:3:175:TYR:CZ	2.50	0.46
2:B:142:ALA:O	2:B:145:TYR:HB2	2.15	0.46
3:H:303:ASP:HB3	3:H:307:ARG:NH2	2.30	0.46
3:M:324:VAL:HG23	3:M:326:VAL:H	1.80	0.46
2:B:75:LEU:HD21	2:B:133:VAL:HG11	1.97	0.46
3:C:255:ASN:OD1	3:C:257:ARG:HG2	2.15	0.46
3:C:306:ILE:HD13	3:C:330:LEU:HD13	1.97	0.46
3:M:350:ASP:C	3:M:371:LEU:HD12	2.36	0.46
3:W:186:THR:HG21	3:W:354:ALA:CB	2.45	0.46
5:Y:61:THR:O	5:Y:65:ILE:HG13	2.15	0.46
5:J:121:ILE:O	5:J:125:ILE:HG12	2.15	0.46
5:O:43:ASP:O	5:O:46:GLU:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:51:LEU:HD23	5:O:51:LEU:HA	1.76	0.46
3:M:96:PRO:HG2	3:R:142:LEU:HD11	1.98	0.46
2:V:142:ALA:O	2:V:145:TYR:HB2	2.16	0.46
3:C:183:THR:HB	3:C:199:ASN:ND2	2.20	0.46
2:V:18:VAL:HG13	2:V:23:VAL:HG21	1.98	0.46
3:2:198:LYS:NZ	3:2:329:ILE:HD11	2.31	0.45
2:B:92:HIS:HA	2:B:96:LEU:HB2	1.97	0.45
3:C:277:VAL:HG12	3:C:278:SER:O	2.17	0.45
3:C:314:VAL:HA	3:C:315:PRO:HD3	1.75	0.45
5:E:49:CYS:HA	5:E:178:LEU:HD21	1.97	0.45
2:L:118:PHE:O	2:L:121:GLU:HB3	2.16	0.45
3:W:96:PRO:HG2	3:2:142:LEU:HD11	1.96	0.45
3:M:114:TYR:CD2	3:M:255:ASN:HA	2.51	0.45
3:W:303:ASP:HB3	3:W:307:ARG:NH2	2.31	0.45
3:W:198:LYS:NZ	3:W:329:ILE:HD11	2.31	0.45
5:J:43:ASP:O	5:J:46:GLU:HG2	2.17	0.45
3:M:373:PHE:CZ	3:M:375:LYS:HB2	2.52	0.45
3:M:376:SER:HB2	3:M:380:ALA:O	2.16	0.45
1:P:83:LEU:HD11	6:P:201:HEM:HMA1	1.97	0.45
1:P:48:LEU:HD23	1:P:48:LEU:HA	1.75	0.45
1:U:9:ASN:ND2	1:U:121:VAL:HG22	2.26	0.45
2:V:75:LEU:HD21	2:V:133:VAL:HG11	1.98	0.45
5:4:39:LEU:HD23	5:4:40:LYS:H	1.81	0.45
3:C:128:ASN:HD22	3:C:130:GLU:HB2	1.80	0.45
3:C:373:PHE:CZ	3:C:375:LYS:HB2	2.51	0.45
5:E:51:LEU:HD23	5:E:51:LEU:HA	1.76	0.45
1:F:48:LEU:HA	1:F:48:LEU:HD23	1.76	0.45
5:J:44:GLU:OE2	5:J:221:GLY:HA3	2.17	0.45
1:K:106:LEU:HA	1:K:106:LEU:HD23	1.82	0.45
3:M:314:VAL:HA	3:M:315:PRO:HD3	1.76	0.45
5:T:39:LEU:HD23	5:T:40:LYS:H	1.81	0.45
5:Y:38:GLY:O	5:Y:39:LEU:HB2	2.17	0.45
1:Z:27:GLU:OE2	1:Z:108:THR:HG23	2.17	0.45
2:1:8:LYS:O	2:1:12:THR:OG1	2.29	0.45
3:2:184:GLY:O	3:2:352:GLY:HA3	2.15	0.45
2:G:69:GLY:O	2:G:72:SER:N	2.50	0.45
4:I:140:THR:OG1	4:I:143:LYS:O	2.31	0.45
3:2:135:ASN:O	3:2:139:GLY:N	2.46	0.45
3:2:303:ASP:HB3	3:2:307:ARG:NH2	2.31	0.45
5:J:39:LEU:HD23	5:J:40:LYS:H	1.81	0.45
2:L:109:VAL:O	2:L:113:VAL:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:92:HIS:HA	2:L:96:LEU:HB2	1.98	0.45
5:O:38:GLY:O	5:O:39:LEU:HB2	2.17	0.45
2:Q:97:HIS:HB3	3:R:163:LEU:HD12	1.98	0.45
3:W:332:GLU:OE2	8:W:1003:NAG:H62	2.16	0.45
3:W:336:CYS:SG	3:W:384:VAL:HG23	2.57	0.45
4:X:126:TYR:CE2	4:X:202:THR:HG21	2.51	0.45
2:L:75:LEU:HD21	2:L:133:VAL:HG11	1.98	0.45
3:M:334:THR:HA	3:M:386:VAL:HA	1.99	0.45
3:R:92:CYS:SG	3:R:92:CYS:O	2.74	0.45
3:2:302:GLN:O	3:2:306:ILE:HG12	2.16	0.45
5:4:126:THR:HG23	5:4:127:SER:H	1.82	0.45
5:E:191:LYS:NZ	5:E:195:GLU:OE2	2.48	0.45
3:H:118:ARG:O	3:H:119:THR:HB	2.17	0.45
3:H:114:TYR:CD2	3:H:255:ASN:HA	2.51	0.45
2:L:142:ALA:O	2:L:145:TYR:HB2	2.17	0.45
3:M:119:THR:HG21	3:M:143:PRO:HB3	1.98	0.45
3:M:312:SER:HB2	3:M:314:VAL:O	2.17	0.45
3:R:135:ASN:O	3:R:139:GLY:N	2.45	0.45
3:R:391:ILE:O	3:R:395:VAL:HG22	2.17	0.45
3:W:153:LYS:HB3	3:W:256:GLU:HB2	1.98	0.45
1:A:107:VAL:HG11	2:B:127:GLN:OE1	2.17	0.45
1:F:99:LYS:HD3	1:F:99:LYS:HA	1.40	0.45
3:H:312:SER:HB2	3:H:314:VAL:O	2.16	0.45
5:J:287:ASN:O	5:J:291:THR:OG1	2.18	0.45
6:L:201:HEM:CBC	6:L:201:HEM:HHD	2.46	0.45
3:M:186:THR:HG21	3:M:354:ALA:CB	2.46	0.45
2:Q:142:ALA:O	2:Q:145:TYR:HB2	2.17	0.45
3:2:312:SER:HB2	3:2:314:VAL:O	2.16	0.45
2:B:98:VAL:O	2:B:145:TYR:OH	2.23	0.45
5:T:287:ASN:O	5:T:291:THR:OG1	2.19	0.45
3:W:170:PRO:HB2	3:W:259:MET:HG2	1.99	0.45
1:U:11:LYS:NZ	4:X:151:ASN:OD1	2.49	0.45
3:2:114:TYR:CD2	3:2:255:ASN:HA	2.52	0.44
2:B:51:PRO:O	2:B:55:MET:HG2	2.17	0.44
3:C:119:THR:HG23	3:C:121:GLY:CA	2.46	0.44
3:H:188:ILE:CG1	3:H:263:LEU:HD11	2.47	0.44
2:L:71:PHE:CE2	2:L:137:VAL:HG11	2.52	0.44
4:N:96:ASP:HB3	4:N:99:LEU:HD22	1.99	0.44
3:R:306:ILE:CD1	3:R:330:LEU:HD13	2.47	0.44
3:W:224:LYS:HE2	3:W:224:LYS:HB3	1.74	0.44
2:1:109:VAL:O	2:1:113:VAL:HG23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:324:VAL:HG23	3:C:326:VAL:H	1.82	0.44
1:F:11:LYS:HE3	4:I:126:TYR:CE1	2.52	0.44
3:M:128:ASN:HD22	3:M:130:GLU:HB2	1.82	0.44
3:R:128:ASN:HD22	3:R:130:GLU:HB2	1.81	0.44
2:1:48:LEU:HA	2:1:48:LEU:HD23	1.85	0.44
2:B:101:GLU:HA	2:B:101:GLU:OE1	2.18	0.44
3:C:107:VAL:HG11	3:H:95:PRO:HG3	2.00	0.44
3:H:162:HIS:HB2	3:H:294:TYR:O	2.16	0.44
1:P:99:LYS:HA	1:P:99:LYS:HD3	1.38	0.44
3:W:374:ASP:OD1	3:W:374:ASP:N	2.35	0.44
5:Y:39:LEU:HD23	5:Y:40:LYS:H	1.83	0.44
3:2:175:MET:HB2	3:2:219:LEU:HD13	1.99	0.44
3:C:186:THR:HG21	3:C:354:ALA:CB	2.46	0.44
4:D:176:SER:HA	4:D:177:PRO:HD3	1.81	0.44
5:E:170:ALA:O	5:E:174:VAL:HG13	2.17	0.44
1:F:127:LYS:O	1:F:130:ALA:HB3	2.17	0.44
3:H:175:MET:HB2	3:H:219:LEU:HD13	1.98	0.44
3:H:277:VAL:O	3:H:294:TYR:HA	2.18	0.44
3:H:334:THR:HA	3:H:386:VAL:HA	2.00	0.44
1:K:101:LEU:HG	1:K:105:LEU:HD12	1.98	0.44
2:L:11:VAL:HA	2:L:130:TYR:HE2	1.82	0.44
3:M:186:THR:HG21	3:M:354:ALA:N	2.33	0.44
1:U:65:ALA:HB2	6:U:201:HEM:HMA1	1.98	0.44
3:W:314:VAL:HA	3:W:315:PRO:HD3	1.77	0.44
2:1:31:LEU:HD13	2:1:106:LEU:HB2	1.99	0.44
5:E:38:GLY:O	5:E:39:LEU:HB2	2.18	0.44
2:G:20:VAL:HA	2:G:68:LEU:HD21	2.00	0.44
3:M:345:ASP:OD1	3:M:346:THR:HG22	2.17	0.44
4:N:131:ILE:HG21	4:N:148:LEU:HD22	1.99	0.44
3:2:336:CYS:SG	3:2:384:VAL:HG23	2.58	0.44
5:4:43:ASP:O	5:4:46:GLU:HG2	2.18	0.44
2:G:8:LYS:O	2:G:12:THR:OG1	2.31	0.44
2:Q:31:LEU:HD13	2:Q:106:LEU:HB2	1.99	0.44
3:R:175:MET:HB2	3:R:219:LEU:HD13	1.99	0.44
1:U:106:LEU:HD23	1:U:106:LEU:HA	1.85	0.44
3:W:174:LYS:HB2	3:W:280:TRP:CG	2.52	0.44
3:W:184:GLY:O	3:W:352:GLY:HA3	2.18	0.44
3:W:388:VAL:O	3:W:391:ILE:HG13	2.18	0.44
3:2:373:PHE:CZ	3:2:375:LYS:HB2	2.52	0.44
2:B:11:VAL:HA	2:B:130:TYR:HE2	1.82	0.44
3:C:345:ASP:OD1	3:C:346:THR:HG22	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:20:VAL:HA	2:Q:68:LEU:HD21	2.00	0.44
2:1:18:VAL:HG13	2:1:23:VAL:HG21	1.99	0.44
3:C:312:SER:HB2	3:C:314:VAL:O	2.18	0.44
2:G:101:GLU:HA	2:G:101:GLU:OE1	2.18	0.44
2:G:51:PRO:O	2:G:55:MET:HG2	2.18	0.44
3:H:206:GLU:HG3	3:H:206:GLU:H	1.62	0.44
3:H:184:GLY:O	3:H:352:GLY:HA3	2.16	0.44
5:J:122:ILE:HD12	5:J:129:ARG:HH12	1.83	0.44
5:J:51:LEU:HD23	5:J:51:LEU:HA	1.73	0.44
2:L:31:LEU:HD13	2:L:106:LEU:HB2	2.00	0.44
8:M:1001:NAG:O7	8:M:1001:NAG:O3	2.34	0.44
2:V:92:HIS:HA	2:V:96:LEU:HB2	1.99	0.44
3:W:340:SER:HB3	3:W:344:GLU:N	2.33	0.44
1:Z:85:ASP:N	1:Z:85:ASP:OD1	2.51	0.44
3:C:143:PRO:HG2	3:H:98:ILE:HD13	2.00	0.44
3:C:306:ILE:CD1	3:C:330:LEU:HD13	2.48	0.44
4:N:99:LEU:HD23	4:N:172:LEU:HD23	2.00	0.44
3:R:376:SER:HB2	3:R:380:ALA:O	2.18	0.44
5:T:170:ALA:O	5:T:174:VAL:HG13	2.18	0.44
3:2:170:PRO:HB2	3:2:259:MET:HG2	2.00	0.43
3:2:174:LYS:HB2	3:2:280:TRP:CG	2.53	0.43
3:2:391:ILE:O	3:2:395:VAL:HG22	2.18	0.43
2:Q:101:GLU:HA	2:Q:101:GLU:OE1	2.17	0.43
2:Q:18:VAL:HG13	2:Q:23:VAL:HG21	1.99	0.43
3:R:118:ARG:O	3:R:119:THR:HB	2.18	0.43
1:U:131:SER:HA	3:W:379:VAL:CG1	2.48	0.43
3:W:391:ILE:O	3:W:395:VAL:HG22	2.18	0.43
3:2:128:ASN:HD22	3:2:130:GLU:HB2	1.82	0.43
3:2:245:LEU:HD11	3:2:395:VAL:HG12	2.00	0.43
3:2:186:THR:HG21	3:2:354:ALA:CB	2.48	0.43
3:C:160:GLY:HA3	3:C:344:GLU:HG2	2.00	0.43
3:C:334:THR:HA	3:C:386:VAL:HA	2.00	0.43
4:I:145:GLU:OE2	4:I:171:ARG:NH2	2.42	0.43
5:J:175:TRP:HA	5:J:178:LEU:HB2	2.00	0.43
5:J:61:THR:O	5:J:65:ILE:HG13	2.19	0.43
5:O:173:ASP:OD2	5:O:229:LYS:NZ	2.51	0.43
3:W:172:GLN:HE21	3:W:173:ALA:N	2.16	0.43
3:H:191:GLN:HB3	3:H:192:TRP:CD1	2.53	0.43
3:H:337:ALA:HB3	3:H:385:TYR:HE1	1.83	0.43
3:H:340:SER:OG	3:H:341:LYS:N	2.51	0.43
2:L:45:PHE:HZ	2:L:63:HIS:ND1	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:296:MET:CE	5:O:71:ARG:HA	2.49	0.43
1:U:83:LEU:HD22	1:U:87:HIS:CE1	2.36	0.43
5:Y:122:ILE:HD12	5:Y:129:ARG:HH12	1.83	0.43
5:4:122:ILE:HD12	5:4:129:ARG:HH12	1.83	0.43
3:H:196:THR:HG21	3:H:351:ALA:HB1	2.00	0.43
3:R:312:SER:HB2	3:R:314:VAL:O	2.17	0.43
5:T:122:ILE:HD12	5:T:129:ARG:HH12	1.83	0.43
5:T:44:GLU:OE2	5:T:221:GLY:HA3	2.18	0.43
1:U:127:LYS:O	1:U:130:ALA:HB3	2.19	0.43
2:V:31:LEU:HD13	2:V:106:LEU:HB2	2.00	0.43
2:1:92:HIS:HA	2:1:96:LEU:HB2	2.00	0.43
1:A:99:LYS:HD3	1:A:99:LYS:HA	1.38	0.43
3:H:183:THR:HB	3:H:199:ASN:ND2	2.20	0.43
2:Q:57:ASN:HB3	2:Q:60:VAL:HG23	2.01	0.43
2:Q:69:GLY:O	2:Q:72:SER:N	2.52	0.43
3:2:206:GLU:HG3	3:2:206:GLU:H	1.62	0.43
3:2:267:ASP:CB	3:2:389:THR:HG21	2.48	0.43
1:A:106:LEU:HD23	1:A:106:LEU:HA	1.85	0.43
1:A:119:PRO:HG2	2:B:55:MET:HG3	2.00	0.43
1:F:27:GLU:OE2	1:F:108:THR:HG23	2.19	0.43
3:M:257:ARG:HG3	3:M:258:VAL:HG23	2.01	0.43
5:O:170:ALA:O	5:O:174:VAL:HG13	2.19	0.43
3:R:181:LEU:HA	3:R:181:LEU:HD23	1.77	0.43
2:V:118:PHE:O	2:V:121:GLU:HB3	2.19	0.43
3:W:135:ASN:O	3:W:139:GLY:N	2.46	0.43
3:W:245:LEU:HD23	3:W:245:LEU:HA	1.63	0.43
3:W:296:MET:CE	5:Y:71:ARG:HA	2.49	0.43
1:Z:35:SER:HB3	2:1:131:GLN:HG3	2.01	0.43
2:1:41:PHE:HB3	6:1:201:HEM:HMD2	2.00	0.43
5:4:170:ALA:O	5:4:174:VAL:HG13	2.18	0.43
3:C:340:SER:OG	3:C:341:LYS:N	2.52	0.43
2:L:69:GLY:O	2:L:72:SER:N	2.51	0.43
3:M:114:TYR:O	3:M:148:VAL:HG23	2.19	0.43
3:M:312:SER:OG	3:M:313:THR:N	2.51	0.43
2:Q:8:LYS:O	2:Q:12:THR:OG1	2.31	0.43
5:Y:206:SER:HA	8:Y:1002:NAG:H62	1.99	0.43
5:Y:46:GLU:HA	5:Y:49:CYS:HB3	1.99	0.43
5:4:210:LEU:O	5:4:214:ILE:HG12	2.19	0.43
1:A:9:ASN:ND2	1:A:121:VAL:HG22	2.29	0.43
3:C:188:ILE:CG1	3:C:263:LEU:HD11	2.48	0.43
3:C:391:ILE:O	3:C:395:VAL:HG22	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:166:LYS:HD2	5:E:232:ASP:HB2	2.01	0.43
2:G:142:ALA:O	2:G:145:TYR:HB2	2.18	0.43
2:G:18:VAL:HG13	2:G:23:VAL:HG21	1.99	0.43
2:G:71:PHE:CE2	2:G:137:VAL:HG11	2.53	0.43
5:J:55:LEU:O	5:J:58:VAL:HG13	2.18	0.43
3:R:162:HIS:HB2	3:R:294:TYR:O	2.18	0.43
3:R:184:GLY:O	3:R:352:GLY:HA3	2.18	0.43
5:T:58:VAL:HG23	5:T:62:LEU:HD12	1.99	0.43
1:U:14:TRP:HE1	1:U:67:THR:HG23	1.83	0.43
3:2:172:GLN:HE21	3:2:173:ALA:N	2.17	0.43
3:2:179:HIS:HB3	8:2:1002:NAG:C8	2.49	0.43
5:4:46:GLU:HA	5:4:49:CYS:HB3	2.01	0.43
2:B:26:GLU:HG3	2:B:55:MET:HE1	2.00	0.43
3:W:350:ASP:C	3:W:371:LEU:HD12	2.39	0.43
1:Z:131:SER:HA	3:2:379:VAL:CG1	2.49	0.43
2:1:118:PHE:O	2:1:121:GLU:HB3	2.18	0.43
3:H:186:THR:HG21	3:H:354:ALA:CB	2.49	0.43
1:K:99:LYS:HA	1:K:99:LYS:HD3	1.40	0.43
3:R:114:TYR:O	3:R:148:VAL:HG23	2.19	0.43
3:R:310:GLU:HA	3:R:319:THR:O	2.19	0.43
5:T:166:LYS:HD2	5:T:232:ASP:HB2	2.00	0.43
5:T:51:LEU:HA	5:T:51:LEU:HD23	1.74	0.43
3:W:306:ILE:CD1	3:W:330:LEU:HD13	2.49	0.43
5:Y:175:TRP:HA	5:Y:178:LEU:HB2	2.01	0.43
5:Y:252:GLY:O	5:Y:256:LYS:HG2	2.19	0.43
5:Y:283:GLU:HG3	5:Y:284:GLU:H	1.83	0.43
2:B:42:PHE:CE2	6:B:201:HEM:HBC2	2.54	0.42
5:E:210:LEU:O	5:E:214:ILE:HG12	2.19	0.42
1:F:14:TRP:HE1	1:F:67:THR:HG23	1.83	0.42
3:H:128:ASN:HD22	3:H:130:GLU:HB2	1.83	0.42
2:L:44:SER:O	5:O:161:SER:OG	2.22	0.42
3:M:118:ARG:O	3:M:119:THR:HB	2.19	0.42
3:R:191:GLN:HB3	3:R:192:TRP:CD1	2.54	0.42
3:R:257:ARG:HG3	3:R:258:VAL:HG23	2.01	0.42
3:R:334:THR:HA	3:R:386:VAL:HA	2.01	0.42
3:R:337:ALA:HB3	3:R:385:TYR:HE1	1.84	0.42
1:Z:127:LYS:O	1:Z:130:ALA:HB3	2.19	0.42
2:1:51:PRO:O	2:1:55:MET:HG2	2.19	0.42
2:B:31:LEU:HD13	2:B:106:LEU:HB2	2.01	0.42
3:C:206:GLU:H	3:C:206:GLU:HG3	1.59	0.42
5:O:250:THR:OG1	5:O:253:ARG:NH1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:O:283:GLU:HG3	5:O:284:GLU:H	1.84	0.42
4:S:195:GLU:OE1	4:S:216:LYS:HE2	2.19	0.42
5:T:175:TRP:HA	5:T:178:LEU:HB2	2.01	0.42
2:V:8:LYS:O	2:V:12:THR:OG1	2.31	0.42
3:C:309:TYR:CD1	3:C:328:PRO:HG3	2.53	0.42
2:G:118:PHE:O	2:G:121:GLU:HB3	2.19	0.42
2:G:63:HIS:O	2:G:67:VAL:HG23	2.19	0.42
2:Q:118:PHE:O	2:Q:121:GLU:HB3	2.19	0.42
3:R:174:LYS:HB2	3:R:280:TRP:CG	2.54	0.42
2:V:70:ALA:HB2	6:V:201:HEM:HMA2	2.01	0.42
5:Y:250:THR:OG1	5:Y:253:ARG:NH1	2.51	0.42
3:2:118:ARG:O	3:2:119:THR:HB	2.20	0.42
2:B:44:SER:O	5:E:161:SER:OG	2.20	0.42
3:C:312:SER:OG	3:C:313:THR:N	2.52	0.42
3:H:391:ILE:O	3:H:395:VAL:HG22	2.19	0.42
5:J:58:VAL:HG23	5:J:62:LEU:HD12	2.00	0.42
3:M:340:SER:OG	3:M:341:LYS:N	2.53	0.42
3:R:186:THR:HG21	3:R:354:ALA:CB	2.49	0.42
3:W:181:LEU:HD23	3:W:181:LEU:HA	1.79	0.42
3:2:160:GLY:HA3	3:2:344:GLU:HB3	2.00	0.42
1:F:9:ASN:ND2	1:F:121:VAL:HG22	2.26	0.42
3:H:277:VAL:HG12	3:H:278:SER:O	2.20	0.42
3:R:179:HIS:HB3	8:R:1002:NAG:H83	2.00	0.42
3:R:119:THR:HG23	3:R:121:GLY:CA	2.50	0.42
3:R:277:VAL:O	3:R:294:TYR:HA	2.20	0.42
5:T:283:GLU:HG3	5:T:284:GLU:H	1.84	0.42
1:U:11:LYS:HE3	4:X:126:TYR:CE1	2.55	0.42
1:U:125:LEU:HA	1:U:125:LEU:HD23	1.85	0.42
1:U:66:LEU:O	1:U:70:VAL:HG12	2.20	0.42
2:1:11:VAL:HA	2:1:130:TYR:HE2	1.84	0.42
3:2:340:SER:OG	3:2:341:LYS:N	2.52	0.42
5:E:58:VAL:HG23	5:E:62:LEU:HD12	1.99	0.42
3:H:267:ASP:CB	3:H:389:THR:HG21	2.49	0.42
5:J:283:GLU:HG3	5:J:284:GLU:H	1.84	0.42
5:T:210:LEU:O	5:T:214:ILE:HG12	2.20	0.42
3:W:196:THR:HG21	3:W:351:ALA:HB1	2.02	0.42
2:B:63:HIS:O	2:B:67:VAL:HG23	2.19	0.42
5:E:122:ILE:HD12	5:E:129:ARG:HH12	1.85	0.42
5:E:39:LEU:CD2	5:E:40:LYS:H	2.33	0.42
2:L:92:HIS:O	2:L:97:HIS:N	2.52	0.42
3:M:225:GLN:OE1	3:M:258:VAL:HG21	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:334:THR:HA	3:W:386:VAL:HA	2.02	0.42
5:Y:44:GLU:OE2	5:Y:221:GLY:HA3	2.20	0.42
2:1:124:PRO:HB2	2:1:125:PRO:HD3	2.02	0.42
1:A:125:LEU:HA	1:A:125:LEU:HD23	1.92	0.42
8:E:1002:NAG:O7	8:E:1002:NAG:C3	2.67	0.42
6:G:201:HEM:HHD	6:G:201:HEM:CBC	2.49	0.42
8:H:1004:NAG:HO3	8:H:1004:NAG:C7	2.28	0.42
3:H:160:GLY:HA3	3:H:344:GLU:HG2	1.99	0.42
3:M:151:LYS:H	3:M:259:MET:HE1	1.83	0.42
1:A:38:THR:O	1:A:41:THR:HG23	2.20	0.42
3:C:200:LEU:HD12	3:C:217:LEU:HD11	2.02	0.42
2:L:98:VAL:O	2:L:145:TYR:OH	2.22	0.42
1:P:127:LYS:O	1:P:130:ALA:HB3	2.19	0.42
1:P:27:GLU:OE2	1:P:108:THR:HG23	2.20	0.42
2:Q:92:HIS:HA	2:Q:96:LEU:HB2	2.01	0.42
3:W:340:SER:OG	3:W:341:LYS:N	2.53	0.42
1:Z:14:TRP:HE1	1:Z:67:THR:HG23	1.85	0.42
1:Z:83:LEU:HD22	1:Z:87:HIS:CE1	2.35	0.42
3:2:188:ILE:CG1	3:2:263:LEU:HD11	2.50	0.42
1:A:48:LEU:HA	1:A:48:LEU:HD23	1.73	0.42
3:C:118:ARG:O	3:C:119:THR:HB	2.20	0.42
3:H:147:ALA:HB1	3:H:254:VAL:HG21	2.02	0.42
2:L:11:VAL:HG13	2:L:130:TYR:CZ	2.55	0.42
5:T:61:THR:O	5:T:65:ILE:HG13	2.20	0.42
5:4:283:GLU:HG3	5:4:284:GLU:H	1.85	0.41
2:B:41:PHE:HB3	6:B:201:HEM:HMD2	2.01	0.41
3:C:198:LYS:HZ1	3:C:329:ILE:HD11	1.84	0.41
5:E:283:GLU:HG3	5:E:284:GLU:H	1.85	0.41
2:G:124:PRO:HB2	2:G:125:PRO:HD3	2.02	0.41
3:H:376:SER:HB2	3:H:380:ALA:O	2.20	0.41
5:J:206:SER:HA	8:J:1002:NAG:O6	2.19	0.41
2:L:20:VAL:HA	2:L:68:LEU:HD21	2.01	0.41
3:M:147:ALA:HB1	3:M:254:VAL:HG21	2.02	0.41
3:R:183:THR:HB	3:R:199:ASN:ND2	2.20	0.41
3:R:267:ASP:CB	3:R:389:THR:HG21	2.50	0.41
3:W:114:TYR:O	3:W:148:VAL:HG23	2.20	0.41
1:Z:99:LYS:HA	1:Z:99:LYS:HD3	1.41	0.41
3:2:350:ASP:C	3:2:371:LEU:HD12	2.41	0.41
3:2:388:VAL:O	3:2:391:ILE:HG13	2.20	0.41
1:A:101:LEU:HG	1:A:105:LEU:HD12	2.01	0.41
5:J:41:THR:OG1	5:J:42:LYS:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:102:ASN:HA	2:L:105:LEU:HB2	2.01	0.41
2:L:124:PRO:HB2	2:L:125:PRO:HD3	2.02	0.41
3:R:119:THR:C	3:R:121:GLY:HA3	2.40	0.41
3:R:198:LYS:NZ	3:R:329:ILE:HD11	2.35	0.41
1:U:109:LEU:HD23	1:U:109:LEU:HA	1.82	0.41
5:Y:210:LEU:O	5:Y:214:ILE:HG12	2.19	0.41
5:4:97:LEU:O	5:4:100:VAL:HG12	2.20	0.41
8:C:1002:NAG:O3	8:C:1003:NAG:N2	2.54	0.41
1:K:32:MET:SD	1:K:101:LEU:HB2	2.60	0.41
6:Q:201:HEM:HBB2	6:Q:201:HEM:CHC	2.39	0.41
3:R:188:ILE:CG1	3:R:263:LEU:HD11	2.50	0.41
5:T:126:THR:HG23	5:T:127:SER:H	1.85	0.41
1:U:46:PHE:HZ	6:U:201:HEM:O1D	2.03	0.41
2:V:71:PHE:CE2	2:V:137:VAL:HG11	2.55	0.41
3:2:163:LEU:HD22	3:2:164:ASP:H	1.85	0.41
5:4:55:LEU:O	5:4:58:VAL:HG13	2.20	0.41
3:C:225:GLN:OE1	3:C:258:VAL:HG21	2.19	0.41
4:D:99:LEU:HD23	4:D:172:LEU:HD23	2.02	0.41
5:E:55:LEU:O	5:E:58:VAL:HG13	2.20	0.41
3:H:212:ASP:N	3:H:212:ASP:OD1	2.53	0.41
5:O:97:LEU:O	5:O:100:VAL:HG12	2.20	0.41
4:X:145:GLU:OE2	4:X:171:ARG:NH2	2.42	0.41
1:Z:9:ASN:ND2	1:Z:121:VAL:HG22	2.26	0.41
2:1:92:HIS:O	2:1:97:HIS:N	2.53	0.41
3:C:174:LYS:HB2	3:C:280:TRP:CG	2.55	0.41
3:C:345:ASP:CG	3:C:346:THR:N	2.69	0.41
1:F:83:LEU:HD22	1:F:87:HIS:CE1	2.36	0.41
1:K:3:SER:N	1:K:6:ASP:OD2	2.44	0.41
3:M:200:LEU:HD12	3:M:217:LEU:HD11	2.02	0.41
8:R:1002:NAG:H3	8:R:1003:NAG:HN2	1.85	0.41
3:M:110:GLN:N	3:R:102:TYR:O	2.40	0.41
3:R:113:ASN:N	3:R:113:ASN:OD1	2.53	0.41
3:R:345:ASP:CG	3:R:346:THR:N	2.70	0.41
4:S:90:LEU:HD22	4:S:156:TRP:HB2	2.02	0.41
1:U:87:HIS:NE2	6:U:201:HEM:NA	2.68	0.41
2:V:41:PHE:HB3	6:V:201:HEM:HMD2	2.02	0.41
3:2:334:THR:HA	3:2:386:VAL:HA	2.03	0.41
3:C:279:GLY:O	3:C:292:LEU:HD12	2.20	0.41
5:E:250:THR:OG1	5:E:253:ARG:NH1	2.50	0.41
2:G:92:HIS:O	2:G:97:HIS:N	2.53	0.41
3:H:174:LYS:HB2	3:H:280:TRP:CG	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:181:LEU:HD23	3:H:181:LEU:HA	1.78	0.41
3:H:225:GLN:OE1	3:H:258:VAL:HG21	2.20	0.41
2:L:63:HIS:O	2:L:67:VAL:HG23	2.20	0.41
3:M:395:VAL:O	3:M:399:ILE:HG12	2.20	0.41
5:O:39:LEU:CD2	5:O:40:LYS:H	2.34	0.41
5:O:44:GLU:OE2	5:O:221:GLY:HA3	2.21	0.41
2:Q:98:VAL:O	2:Q:145:TYR:OH	2.21	0.41
1:U:83:LEU:HD23	1:U:83:LEU:HA	1.95	0.41
2:V:98:VAL:O	2:V:145:TYR:OH	2.26	0.41
3:W:160:GLY:HA3	3:W:344:GLU:HG2	2.03	0.41
3:W:373:PHE:CZ	3:W:375:LYS:HB2	2.56	0.41
5:Y:39:LEU:CD2	5:Y:40:LYS:H	2.34	0.41
1:Z:107:VAL:HG11	2:1:127:GLN:OE1	2.19	0.41
2:1:142:ALA:O	2:1:145:TYR:HB2	2.20	0.41
5:4:76:VAL:HG13	5:4:146:ARG:HG3	2.03	0.41
6:A:201:HEM:HBB2	6:A:201:HEM:HMB1	2.03	0.41
2:B:118:PHE:O	2:B:121:GLU:HB3	2.21	0.41
8:J:1002:NAG:O3	8:J:1002:NAG:O7	2.37	0.41
5:O:42:LYS:HG2	5:O:42:LYS:O	2.20	0.41
3:R:147:ALA:HB1	3:R:254:VAL:HG21	2.03	0.41
2:V:105:LEU:HA	2:V:105:LEU:HD23	1.92	0.41
2:V:11:VAL:HA	2:V:130:TYR:HE2	1.86	0.41
3:W:395:VAL:O	3:W:399:ILE:HG12	2.20	0.41
5:Y:226:HIS:HB3	5:Y:229:LYS:HE2	2.02	0.41
3:2:345:ASP:OD1	3:2:346:THR:HG22	2.21	0.41
5:E:44:GLU:OE2	5:E:221:GLY:HA3	2.21	0.41
5:J:39:LEU:H	5:J:223:LEU:HD21	1.84	0.41
1:K:11:LYS:HE3	4:N:126:TYR:CE1	2.56	0.41
5:O:122:ILE:HD12	5:O:129:ARG:HH12	1.86	0.41
5:O:46:GLU:HA	5:O:49:CYS:HB3	2.02	0.41
4:S:140:THR:OG1	4:S:143:LYS:O	2.35	0.41
5:T:126:THR:HG23	5:T:127:SER:N	2.36	0.41
6:U:201:HEM:HMB2	6:U:201:HEM:HBB2	2.01	0.41
5:Y:126:THR:HG23	5:Y:127:SER:H	1.85	0.41
4:3:140:THR:OG1	4:3:143:LYS:O	2.35	0.41
3:C:395:VAL:O	3:C:399:ILE:HG12	2.20	0.41
1:K:125:LEU:HA	1:K:125:LEU:HD23	1.87	0.41
1:K:14:TRP:HE1	1:K:67:THR:HG23	1.86	0.41
3:M:309:TYR:CD1	3:M:328:PRO:HG3	2.55	0.41
8:O:1002:NAG:O3	8:O:1002:NAG:O7	2.32	0.41
4:X:99:LEU:HD23	4:X:172:LEU:HD23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:306:ILE:CD1	3:2:330:LEU:HD13	2.49	0.41
5:4:58:VAL:HG23	5:4:62:LEU:HD12	2.02	0.41
5:E:56:LYS:HA	5:E:56:LYS:HE2	2.03	0.41
5:J:56:LYS:HE2	5:J:56:LYS:HA	2.03	0.41
1:K:119:PRO:HG2	2:L:55:MET:HG3	2.02	0.41
1:K:48:LEU:HD23	1:K:48:LEU:HA	1.75	0.41
3:M:273:ARG:HG2	3:M:273:ARG:HH11	1.85	0.41
2:Q:124:PRO:HB2	2:Q:125:PRO:HD3	2.03	0.41
3:R:212:ASP:N	3:R:212:ASP:OD1	2.54	0.41
3:W:206:GLU:HG3	3:W:206:GLU:H	1.62	0.41
5:Y:126:THR:HG23	5:Y:127:SER:N	2.36	0.41
5:4:61:THR:O	5:4:65:ILE:HG13	2.21	0.41
1:A:127:LYS:O	1:A:130:ALA:HB3	2.21	0.41
3:C:151:LYS:H	3:C:259:MET:HE1	1.84	0.41
5:E:226:HIS:HB3	5:E:229:LYS:HE2	2.03	0.41
3:H:119:THR:HG23	3:H:121:GLY:CA	2.48	0.41
3:H:194:LEU:HD13	3:H:370:ILE:HG13	2.03	0.41
3:H:257:ARG:HG3	3:H:258:VAL:HG23	2.03	0.41
2:L:8:LYS:O	2:L:12:THR:OG1	2.30	0.41
3:M:206:GLU:H	3:M:206:GLU:HG3	1.61	0.41
2:Q:51:PRO:O	2:Q:55:MET:HG2	2.21	0.41
2:V:20:VAL:HA	2:V:68:LEU:HD21	2.02	0.41
3:W:191:GLN:HB3	3:W:192:TRP:CD1	2.56	0.41
3:W:269:ALA:O	3:W:299:VAL:HG21	2.21	0.41
5:Y:173:ASP:OD2	5:Y:229:LYS:NZ	2.54	0.41
3:2:314:VAL:HA	3:2:315:PRO:HD3	1.78	0.40
5:4:126:THR:HG23	5:4:127:SER:N	2.37	0.40
2:B:48:LEU:CD2	2:B:54:VAL:HG22	2.51	0.40
3:C:175:MET:HB2	3:C:219:LEU:HD13	2.01	0.40
5:J:97:LEU:O	5:J:100:VAL:HG12	2.21	0.40
5:J:126:THR:HG23	5:J:127:SER:H	1.86	0.40
5:O:70:GLU:O	5:O:74:VAL:HG13	2.21	0.40
2:Q:26:GLU:HA	2:Q:55:MET:HE1	2.03	0.40
1:P:11:LYS:NZ	4:S:151:ASN:OD1	2.49	0.40
5:Y:40:LYS:HG2	5:Y:41:THR:H	1.85	0.40
6:1:201:HEM:HHH	6:1:201:HEM:CBC	2.50	0.40
3:2:114:TYR:O	3:2:148:VAL:HG23	2.21	0.40
3:2:179:HIS:CE1	3:2:203:ASN:HB2	2.56	0.40
3:2:277:VAL:O	3:2:294:TYR:HA	2.21	0.40
5:4:44:GLU:OE2	5:4:221:GLY:HA3	2.21	0.40
5:E:40:LYS:HG2	5:E:41:THR:H	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:106:LEU:HA	1:F:106:LEU:HD23	1.85	0.40
2:G:92:HIS:HA	2:G:96:LEU:HB2	2.02	0.40
3:H:312:SER:OG	3:H:313:THR:N	2.54	0.40
5:J:68:THR:HG22	5:J:69:THR:HG23	2.02	0.40
3:W:200:LEU:HD12	3:W:217:LEU:HD11	2.04	0.40
5:Y:256:LYS:HE3	5:Y:256:LYS:HB3	1.80	0.40
1:Z:38:THR:O	1:Z:41:THR:HG23	2.20	0.40
2:1:20:VAL:HA	2:1:68:LEU:HD21	2.04	0.40
5:4:39:LEU:H	5:4:223:LEU:HD21	1.85	0.40
1:A:83:LEU:HA	1:A:83:LEU:HD23	1.96	0.40
3:C:150:GLY:HA2	3:C:365:TRP:HB2	2.03	0.40
3:H:198:LYS:NZ	3:H:329:ILE:HD11	2.36	0.40
1:P:35:SER:HB3	2:Q:131:GLN:HG3	2.04	0.40
1:P:85:ASP:N	1:P:85:ASP:OD1	2.54	0.40
2:Q:48:LEU:CD2	2:Q:54:VAL:HG22	2.51	0.40
3:R:277:VAL:HG12	3:R:278:SER:O	2.21	0.40
2:V:25:GLY:HA3	2:V:61:LYS:HA	2.03	0.40
3:W:340:SER:HB3	3:W:344:GLU:H	1.84	0.40
3:2:273:ARG:HG2	3:2:273:ARG:HH11	1.86	0.40
5:4:175:TRP:HA	5:4:178:LEU:HB2	2.03	0.40
5:4:256:LYS:HE3	5:4:260:LYS:HE3	2.03	0.40
1:A:35:SER:HB3	2:B:131:GLN:HG3	2.03	0.40
2:B:92:HIS:O	2:B:97:HIS:N	2.54	0.40
3:C:191:GLN:HB3	3:C:192:TRP:CD1	2.57	0.40
1:A:11:LYS:HE3	4:D:126:TYR:CE1	2.56	0.40
5:E:42:LYS:O	5:E:42:LYS:HG2	2.21	0.40
5:J:126:THR:HG23	5:J:127:SER:N	2.37	0.40
1:K:38:THR:O	1:K:41:THR:HG23	2.21	0.40
3:R:395:VAL:O	3:R:399:ILE:HG12	2.21	0.40
5:T:80:LYS:HB2	5:T:146:ARG:NE	2.36	0.40
2:V:104:ARG:HB3	2:V:104:ARG:HE	1.68	0.40
5:Y:170:ALA:O	5:Y:174:VAL:HG13	2.21	0.40
3:2:92:CYS:O	3:2:92:CYS:SG	2.79	0.40
2:B:11:VAL:HG13	2:B:130:TYR:CZ	2.57	0.40
1:K:131:SER:HA	3:M:379:VAL:CG1	2.52	0.40
3:M:371:LEU:HA	3:M:385:TYR:CD2	2.57	0.40
5:O:40:LYS:HG2	5:O:41:THR:H	1.86	0.40
5:T:226:HIS:HB3	5:T:229:LYS:HE2	2.04	0.40
5:T:55:LEU:O	5:T:58:VAL:HG13	2.21	0.40
1:U:85:ASP:OD1	1:U:85:ASP:N	2.54	0.40
2:V:24:GLY:N	2:V:68:LEU:HD22	2.26	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:119:THR:HG23	3:W:121:GLY:CA	2.51	0.40
3:W:273:ARG:HG2	3:W:273:ARG:HH11	1.86	0.40
5:Y:283:GLU:HG3	5:Y:284:GLU:N	2.37	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	139/141 (99%)	130 (94%)	9 (6%)	0	100	100
1	F	139/141 (99%)	129 (93%)	10 (7%)	0	100	100
1	K	139/141 (99%)	129 (93%)	10 (7%)	0	100	100
1	P	139/141 (99%)	128 (92%)	11 (8%)	0	100	100
1	U	139/141 (99%)	130 (94%)	9 (6%)	0	100	100
1	Z	139/141 (99%)	128 (92%)	11 (8%)	0	100	100
2	1	144/146 (99%)	141 (98%)	3 (2%)	0	100	100
2	B	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
2	G	144/146 (99%)	140 (97%)	4 (3%)	0	100	100
2	L	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
2	Q	144/146 (99%)	141 (98%)	3 (2%)	0	100	100
2	V	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
3	2	306/315 (97%)	283 (92%)	23 (8%)	0	100	100
3	C	306/315 (97%)	285 (93%)	21 (7%)	0	100	100
3	H	306/315 (97%)	283 (92%)	23 (8%)	0	100	100
3	M	306/315 (97%)	282 (92%)	24 (8%)	0	100	100
3	R	306/315 (97%)	283 (92%)	23 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	W	306/315 (97%)	283 (92%)	23 (8%)	0	100	100
4	3	142/146 (97%)	135 (95%)	7 (5%)	0	100	100
4	D	142/146 (97%)	134 (94%)	8 (6%)	0	100	100
4	I	142/146 (97%)	135 (95%)	7 (5%)	0	100	100
4	N	142/146 (97%)	134 (94%)	8 (6%)	0	100	100
4	S	142/146 (97%)	134 (94%)	8 (6%)	0	100	100
4	X	142/146 (97%)	135 (95%)	7 (5%)	0	100	100
5	4	259/343 (76%)	232 (90%)	26 (10%)	1 (0%)	38	75
5	E	259/343 (76%)	231 (89%)	27 (10%)	1 (0%)	38	75
5	J	259/343 (76%)	234 (90%)	24 (9%)	1 (0%)	38	75
5	O	259/343 (76%)	232 (90%)	26 (10%)	1 (0%)	38	75
5	T	259/343 (76%)	233 (90%)	25 (10%)	1 (0%)	38	75
5	Y	259/343 (76%)	232 (90%)	26 (10%)	1 (0%)	38	75
All	All	5940/6546 (91%)	5522 (93%)	412 (7%)	6 (0%)	55	88

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	39	LEU
5	J	39	LEU
5	O	39	LEU
5	T	39	LEU
5	Y	39	LEU
5	4	39	LEU

### 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	113/113 (100%)	100 (88%)	13 (12%)	6	27
1	F	113/113 (100%)	100 (88%)	13 (12%)	6	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	113/113 (100%)	100 (88%)	13 (12%)	6	27
1	P	113/113 (100%)	100 (88%)	13 (12%)	6	27
1	U	113/113 (100%)	101 (89%)	12 (11%)	8	30
1	Z	113/113 (100%)	100 (88%)	13 (12%)	6	27
2	1	118/118 (100%)	106 (90%)	12 (10%)	8	32
2	B	118/118 (100%)	107 (91%)	11 (9%)	10	38
2	G	118/118 (100%)	107 (91%)	11 (9%)	10	38
2	L	118/118 (100%)	106 (90%)	12 (10%)	8	32
2	Q	118/118 (100%)	108 (92%)	10 (8%)	12	44
2	V	118/118 (100%)	106 (90%)	12 (10%)	8	32
3	2	266/271 (98%)	238 (90%)	28 (10%)	8	31
3	C	266/271 (98%)	237 (89%)	29 (11%)	7	30
3	H	266/271 (98%)	237 (89%)	29 (11%)	7	30
3	M	266/271 (98%)	235 (88%)	31 (12%)	6	26
3	R	266/271 (98%)	235 (88%)	31 (12%)	6	26
3	W	266/271 (98%)	236 (89%)	30 (11%)	7	28
4	3	133/134 (99%)	129 (97%)	4 (3%)	46	79
4	D	133/134 (99%)	129 (97%)	4 (3%)	46	79
4	I	133/134 (99%)	127 (96%)	6 (4%)	32	68
4	N	133/134 (99%)	129 (97%)	4 (3%)	46	79
4	S	133/134 (99%)	128 (96%)	5 (4%)	38	74
4	X	133/134 (99%)	128 (96%)	5 (4%)	38	74
5	4	202/272 (74%)	180 (89%)	22 (11%)	7	30
5	E	202/272 (74%)	178 (88%)	24 (12%)	6	25
5	J	202/272 (74%)	180 (89%)	22 (11%)	7	30
5	O	202/272 (74%)	179 (89%)	23 (11%)	7	27
5	T	202/272 (74%)	180 (89%)	22 (11%)	7	30
5	Y	202/272 (74%)	180 (89%)	22 (11%)	7	30
All	All	4992/5448 (92%)	4506 (90%)	486 (10%)	9	35

All (486) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	VAL
1	A	23	GLU
1	A	38	THR
1	A	45	HIS
1	A	50	HIS
1	A	67	THR
1	A	70	VAL
1	A	72	HIS
1	A	76	MET
1	A	80	LEU
1	A	92	ARG
1	A	124	SER
1	A	133	SER
2	B	3	LEU
2	B	4	THR
2	B	6	GLU
2	B	12	THR
2	B	22	GLU
2	B	50	THR
2	B	87	THR
2	B	95	LYS
2	B	104	ARG
2	B	145	TYR
2	B	146	HIS
3	C	97	GLU
3	C	120	GLU
3	C	122	ASP
3	C	130	GLU
3	C	148	VAL
3	C	154	ASN
3	C	166	LYS
3	C	176	VAL
3	C	179	HIS
3	C	188	ILE
3	C	191	GLN
3	C	193	LEU
3	C	200	LEU
3	C	221	VAL
3	C	224	LYS
3	C	253	SER
3	C	259	MET
3	C	268	TYR
3	C	278	SER

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Mol	Chain	Res	Type
3	C	297	LEU
3	C	314	VAL
3	C	323	PRO
3	C	326	VAL
3	C	340	SER
3	C	362	GLU
3	C	368	THR
3	C	386	VAL
3	C	388	VAL
3	C	395	VAL
4	D	99	LEU
4	D	171	ARG
4	D	189	VAL
4	D	217	LEU
5	E	37	GLU
5	E	39	LEU
5	E	41	THR
5	E	46	GLU
5	E	51	LEU
5	E	56	LYS
5	E	58	VAL
5	E	68	THR
5	E	76	VAL
5	E	97	LEU
5	E	106	ARG
5	E	107	LEU
5	E	142	VAL
5	E	153	ARG
5	E	174	VAL
5	E	178	LEU
5	E	190	VAL
5	E	205	THR
5	E	206	SER
5	E	210	LEU
5	E	233	VAL
5	E	237	PHE
5	E	243	SER
5	E	282	ILE
1	F	1	VAL
1	F	23	GLU
1	F	38	THR
1	F	45	HIS

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Mol	Chain	Res	Type
1	F	50	HIS
1	F	67	THR
1	F	70	VAL
1	F	72	HIS
1	F	76	MET
1	F	80	LEU
1	F	92	ARG
1	F	124	SER
1	F	133	SER
2	G	3	LEU
2	G	4	THR
2	G	6	GLU
2	G	12	THR
2	G	31	LEU
2	G	50	THR
2	G	87	THR
2	G	95	LYS
2	G	104	ARG
2	G	145	TYR
2	G	146	HIS
3	H	97	GLU
3	H	120	GLU
3	H	122	ASP
3	H	130	GLU
3	H	148	VAL
3	H	154	ASN
3	H	166	LYS
3	H	176	VAL
3	H	179	HIS
3	H	188	ILE
3	H	191	GLN
3	H	193	LEU
3	H	200	LEU
3	H	221	VAL
3	H	224	LYS
3	H	253	SER
3	H	259	MET
3	H	268	TYR
3	H	278	SER
3	H	297	LEU
3	H	314	VAL
3	H	326	VAL

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Mol	Chain	Res	Type
3	H	340	SER
3	H	347	CYS
3	H	357	VAL
3	H	368	THR
3	H	371	LEU
3	H	386	VAL
3	H	388	VAL
4	I	90	LEU
4	I	99	LEU
4	I	113	ASN
4	I	171	ARG
4	I	189	VAL
4	I	217	LEU
5	J	37	GLU
5	J	39	LEU
5	J	41	THR
5	J	51	LEU
5	J	56	LYS
5	J	58	VAL
5	J	68	THR
5	J	76	VAL
5	J	97	LEU
5	J	106	ARG
5	J	142	VAL
5	J	153	ARG
5	J	174	VAL
5	J	178	LEU
5	J	190	VAL
5	J	205	THR
5	J	206	SER
5	J	210	LEU
5	J	233	VAL
5	J	237	PHE
5	J	243	SER
5	J	282	ILE
1	K	1	VAL
1	K	23	GLU
1	K	38	THR
1	K	45	HIS
1	K	50	HIS
1	K	67	THR
1	K	70	VAL

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Mol	Chain	Res	Type
1	K	72	HIS
1	K	76	MET
1	K	80	LEU
1	K	92	ARG
1	K	124	SER
1	K	133	SER
2	L	3	LEU
2	L	4	THR
2	L	6	GLU
2	L	12	THR
2	L	22	GLU
2	L	31	LEU
2	L	50	THR
2	L	87	THR
2	L	95	LYS
2	L	104	ARG
2	L	145	TYR
2	L	146	HIS
3	M	97	GLU
3	M	103	VAL
3	M	120	GLU
3	M	122	ASP
3	M	130	GLU
3	M	148	VAL
3	M	154	ASN
3	M	157	ASN
3	M	166	LYS
3	M	176	VAL
3	M	179	HIS
3	M	191	GLN
3	M	193	LEU
3	M	200	LEU
3	M	221	VAL
3	M	224	LYS
3	M	253	SER
3	M	259	MET
3	M	268	TYR
3	M	278	SER
3	M	297	LEU
3	M	314	VAL
3	M	323	PRO
3	M	326	VAL

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Mol	Chain	Res	Type
3	M	347	CYS
3	M	357	VAL
3	M	362	GLU
3	M	368	THR
3	M	371	LEU
3	M	386	VAL
3	M	388	VAL
4	N	99	LEU
4	N	171	ARG
4	N	189	VAL
4	N	217	LEU
5	O	37	GLU
5	O	39	LEU
5	O	41	THR
5	O	51	LEU
5	O	56	LYS
5	O	58	VAL
5	O	68	THR
5	O	76	VAL
5	O	97	LEU
5	O	106	ARG
5	O	107	LEU
5	O	142	VAL
5	O	153	ARG
5	O	174	VAL
5	O	178	LEU
5	O	190	VAL
5	O	205	THR
5	O	206	SER
5	O	210	LEU
5	O	233	VAL
5	O	237	PHE
5	O	243	SER
5	O	282	ILE
1	P	1	VAL
1	P	23	GLU
1	P	38	THR
1	P	45	HIS
1	P	50	HIS
1	P	67	THR
1	P	70	VAL
1	P	72	HIS

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Mol	Chain	Res	Type
1	P	76	MET
1	P	80	LEU
1	P	92	ARG
1	P	124	SER
1	P	133	SER
2	Q	3	LEU
2	Q	4	THR
2	Q	6	GLU
2	Q	12	THR
2	Q	50	THR
2	Q	87	THR
2	Q	95	LYS
2	Q	104	ARG
2	Q	145	TYR
2	Q	146	HIS
3	R	97	GLU
3	R	120	GLU
3	R	122	ASP
3	R	130	GLU
3	R	148	VAL
3	R	154	ASN
3	R	157	ASN
3	R	166	LYS
3	R	176	VAL
3	R	179	HIS
3	R	191	GLN
3	R	193	LEU
3	R	200	LEU
3	R	221	VAL
3	R	224	LYS
3	R	253	SER
3	R	259	MET
3	R	268	TYR
3	R	278	SER
3	R	297	LEU
3	R	314	VAL
3	R	326	VAL
3	R	340	SER
3	R	347	CYS
3	R	357	VAL
3	R	362	GLU
3	R	368	THR

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Mol	Chain	Res	Type
3	R	371	LEU
3	R	386	VAL
3	R	388	VAL
3	R	395	VAL
4	S	99	LEU
4	S	117	LEU
4	S	171	ARG
4	S	189	VAL
4	S	217	LEU
5	T	37	GLU
5	T	39	LEU
5	T	41	THR
5	T	51	LEU
5	T	56	LYS
5	T	58	VAL
5	T	68	THR
5	T	76	VAL
5	T	97	LEU
5	T	106	ARG
5	T	142	VAL
5	T	153	ARG
5	T	174	VAL
5	T	178	LEU
5	T	190	VAL
5	T	205	THR
5	T	206	SER
5	T	210	LEU
5	T	233	VAL
5	T	237	PHE
5	T	243	SER
5	T	282	ILE
1	U	23	GLU
1	U	38	THR
1	U	45	HIS
1	U	50	HIS
1	U	67	THR
1	U	70	VAL
1	U	72	HIS
1	U	76	MET
1	U	80	LEU
1	U	92	ARG
1	U	124	SER

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Mol	Chain	Res	Type
1	U	133	SER
2	V	3	LEU
2	V	4	THR
2	V	6	GLU
2	V	12	THR
2	V	22	GLU
2	V	31	LEU
2	V	50	THR
2	V	87	THR
2	V	95	LYS
2	V	104	ARG
2	V	145	TYR
2	V	146	HIS
3	W	97	GLU
3	W	120	GLU
3	W	122	ASP
3	W	127	LEU
3	W	130	GLU
3	W	148	VAL
3	W	154	ASN
3	W	166	LYS
3	W	176	VAL
3	W	179	HIS
3	W	188	ILE
3	W	191	GLN
3	W	193	LEU
3	W	200	LEU
3	W	221	VAL
3	W	224	LYS
3	W	253	SER
3	W	259	MET
3	W	268	TYR
3	W	278	SER
3	W	297	LEU
3	W	314	VAL
3	W	326	VAL
3	W	340	SER
3	W	347	CYS
3	W	362	GLU
3	W	368	THR
3	W	371	LEU
3	W	386	VAL

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Mol	Chain	Res	Type
3	W	388	VAL
4	X	99	LEU
4	X	117	LEU
4	X	171	ARG
4	X	189	VAL
4	X	217	LEU
5	Y	37	GLU
5	Y	39	LEU
5	Y	41	THR
5	Y	51	LEU
5	Y	56	LYS
5	Y	58	VAL
5	Y	68	THR
5	Y	76	VAL
5	Y	97	LEU
5	Y	106	ARG
5	Y	142	VAL
5	Y	153	ARG
5	Y	174	VAL
5	Y	178	LEU
5	Y	190	VAL
5	Y	205	THR
5	Y	206	SER
5	Y	210	LEU
5	Y	233	VAL
5	Y	237	PHE
5	Y	243	SER
5	Y	282	ILE
1	Z	1	VAL
1	Z	23	GLU
1	Z	38	THR
1	Z	45	HIS
1	Z	50	HIS
1	Z	67	THR
1	Z	70	VAL
1	Z	72	HIS
1	Z	76	MET
1	Z	80	LEU
1	Z	92	ARG
1	Z	124	SER
1	Z	133	SER
2	1	3	LEU

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Mol	Chain	Res	Type
2	1	4	THR
2	1	6	GLU
2	1	12	THR
2	1	22	GLU
2	1	31	LEU
2	1	50	THR
2	1	87	THR
2	1	95	LYS
2	1	104	ARG
2	1	145	TYR
2	1	146	HIS
3	2	97	GLU
3	2	120	GLU
3	2	122	ASP
3	2	130	GLU
3	2	148	VAL
3	2	154	ASN
3	2	166	LYS
3	2	176	VAL
3	2	179	HIS
3	2	191	GLN
3	2	193	LEU
3	2	200	LEU
3	2	221	VAL
3	2	224	LYS
3	2	253	SER
3	2	259	MET
3	2	268	TYR
3	2	278	SER
3	2	297	LEU
3	2	314	VAL
3	2	326	VAL
3	2	340	SER
3	2	347	CYS
3	2	357	VAL
3	2	368	THR
3	2	371	LEU
3	2	386	VAL
3	2	388	VAL
4	3	99	LEU
4	3	171	ARG
4	3	189	VAL

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Mol	Chain	Res	Type
4	3	217	LEU
5	4	37	GLU
5	4	39	LEU
5	4	41	THR
5	4	51	LEU
5	4	56	LYS
5	4	58	VAL
5	4	68	THR
5	4	76	VAL
5	4	97	LEU
5	4	106	ARG
5	4	142	VAL
5	4	153	ARG
5	4	174	VAL
5	4	178	LEU
5	4	190	VAL
5	4	205	THR
5	4	206	SER
5	4	210	LEU
5	4	233	VAL
5	4	237	PHE
5	4	243	SER
5	4	282	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
2	B	131	GLN
3	C	327	GLN
4	D	113	ASN
5	E	54	GLN
1	F	9	ASN
2	G	131	GLN
3	H	100	HIS
3	H	157	ASN
3	H	327	GLN
3	H	358	HIS
5	J	54	GLN
1	K	9	ASN
3	M	157	ASN
3	M	327	GLN

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Mol	Chain	Res	Type
4	N	113	ASN
5	O	54	GLN
1	P	9	ASN
2	Q	131	GLN
3	R	100	HIS
3	R	327	GLN
4	S	113	ASN
5	T	54	GLN
1	U	9	ASN
3	W	172	GLN
3	W	327	GLN
4	X	165	ASN
5	Y	54	GLN
1	Z	9	ASN
2	1	131	GLN
3	2	100	HIS
3	2	327	GLN
5	4	54	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

67 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	$\# Z  > 2$
6	HEM	1	201	2,7	28,50,50	2.58	8 (28%)	17,82,82	1.97	6 (35%)
7	OXY	1	202	6	1,1,1	0.31	0	0,0,0	0.00	-
8	NAG	2	1001	3	14,14,15	0.25	0	15,19,21	0.60	0
8	NAG	2	1002	8,3	14,14,15	0.35	0	15,19,21	1.37	1 (6%)
8	NAG	2	1003	8	14,14,15	0.80	1 (7%)	15,19,21	0.93	1 (6%)
8	NAG	2	1004	8,3	14,14,15	0.82	1 (7%)	15,19,21	1.87	5 (33%)
8	NAG	2	1005	8	14,14,15	0.51	0	15,19,21	0.92	1 (6%)
8	NAG	4	1001	5	14,14,15	0.19	0	15,19,21	0.56	0
8	NAG	4	1002	5	14,14,15	0.82	1 (7%)	15,19,21	0.73	0
6	HEM	A	201	1,7	28,50,50	2.06	5 (17%)	17,82,82	1.82	5 (29%)
7	OXY	A	202	6	1,1,1	0.26	0	0,0,0	0.00	-
6	HEM	B	201	2,7	28,50,50	2.39	7 (25%)	17,82,82	2.33	5 (29%)
7	OXY	B	202	6	1,1,1	0.27	0	0,0,0	0.00	-
8	NAG	C	1001	3	14,14,15	0.44	0	15,19,21	0.63	0
8	NAG	C	1002	8,3	14,14,15	1.11	1 (7%)	15,19,21	1.83	2 (13%)
8	NAG	C	1003	8	14,14,15	1.13	2 (14%)	15,19,21	1.28	1 (6%)
8	NAG	C	1004	3	14,14,15	1.08	1 (7%)	15,19,21	1.06	1 (6%)
8	NAG	C	1005	8,3	14,14,15	0.60	0	15,19,21	2.13	5 (33%)
8	NAG	C	1006	8	14,14,15	0.23	0	15,19,21	0.67	0
8	NAG	E	1001	5	14,14,15	0.32	0	15,19,21	0.58	0
8	NAG	E	1002	5	14,14,15	0.73	1 (7%)	15,19,21	1.21	1 (6%)
6	HEM	F	201	1,7	28,50,50	2.19	7 (25%)	17,82,82	1.92	4 (23%)
7	OXY	F	202	6	1,1,1	0.24	0	0,0,0	0.00	-
6	HEM	G	201	2,7	28,50,50	2.50	8 (28%)	17,82,82	2.00	7 (41%)
7	OXY	G	202	6	1,1,1	0.27	0	0,0,0	0.00	-
8	NAG	H	1001	3	14,14,15	0.67	1 (7%)	15,19,21	0.70	0
8	NAG	H	1002	3	14,14,15	0.60	0	15,19,21	0.68	0
8	NAG	H	1003	8,3	14,14,15	0.99	1 (7%)	15,19,21	2.11	5 (33%)
8	NAG	H	1004	8	14,14,15	0.57	0	15,19,21	0.88	1 (6%)
8	NAG	J	1001	5	14,14,15	0.38	0	15,19,21	0.58	0
8	NAG	J	1002	5	14,14,15	0.67	1 (7%)	15,19,21	0.53	0
6	HEM	K	201	1,7	28,50,50	2.18	7 (25%)	17,82,82	2.38	7 (41%)
7	OXY	K	202	6	1,1,1	0.24	0	0,0,0	0.00	-
6	HEM	L	201	2,7	28,50,50	2.42	9 (32%)	17,82,82	2.53	8 (47%)
7	OXY	L	202	6	1,1,1	0.29	0	0,0,0	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	NAG	M	1001	3	14,14,15	0.92	1 (7%)	15,19,21	0.88	1 (6%)
8	NAG	M	1002	8,3	14,14,15	0.50	0	15,19,21	2.08	1 (6%)
8	NAG	M	1003	8	14,14,15	1.19	2 (14%)	15,19,21	1.21	1 (6%)
8	NAG	M	1004	3	14,14,15	1.15	1 (7%)	15,19,21	1.00	1 (6%)
8	NAG	M	1005	8,3	14,14,15	0.96	1 (7%)	15,19,21	1.76	5 (33%)
8	NAG	M	1006	8	14,14,15	0.33	0	15,19,21	0.81	1 (6%)
8	NAG	O	1001	5	14,14,15	0.20	0	15,19,21	0.60	0
8	NAG	O	1002	5	14,14,15	0.95	1 (7%)	15,19,21	0.78	0
6	HEM	P	201	1,7	28,50,50	2.11	7 (25%)	17,82,82	1.84	4 (23%)
7	OXY	P	202	6	1,1,1	0.28	0	0,0,0	0.00	-
6	HEM	Q	201	2,7	28,50,50	2.45	6 (21%)	17,82,82	2.25	6 (35%)
7	OXY	Q	202	6	1,1,1	0.26	0	0,0,0	0.00	-
8	NAG	R	1001	3	14,14,15	0.40	0	15,19,21	0.52	0
8	NAG	R	1002	8,3	14,14,15	0.53	0	15,19,21	1.58	1 (6%)
8	NAG	R	1003	8	14,14,15	1.27	2 (14%)	15,19,21	1.22	1 (6%)
8	NAG	R	1004	3	14,14,15	0.37	0	15,19,21	0.51	0
8	NAG	R	1005	8,3	14,14,15	0.82	1 (7%)	15,19,21	1.70	4 (26%)
8	NAG	R	1006	8	14,14,15	0.54	0	15,19,21	0.87	1 (6%)
8	NAG	T	1001	5	14,14,15	0.25	0	15,19,21	0.47	0
8	NAG	T	1002	5	14,14,15	0.61	1 (7%)	15,19,21	1.10	1 (6%)
6	HEM	U	201	1,7	28,50,50	2.23	6 (21%)	17,82,82	1.52	3 (17%)
7	OXY	U	202	6	1,1,1	0.29	0	0,0,0	0.00	-
6	HEM	V	201	2,7	28,50,50	2.44	7 (25%)	17,82,82	1.78	3 (17%)
7	OXY	V	202	6	1,1,1	0.30	0	0,0,0	0.00	-
8	NAG	W	1001	3	14,14,15	0.62	0	15,19,21	0.47	0
8	NAG	W	1002	3	14,14,15	0.51	0	15,19,21	1.44	1 (6%)
8	NAG	W	1003	8,3	14,14,15	0.78	1 (7%)	15,19,21	2.03	5 (33%)
8	NAG	W	1004	8	14,14,15	0.34	0	15,19,21	0.82	1 (6%)
8	NAG	Y	1001	5	14,14,15	0.38	0	15,19,21	0.53	0
8	NAG	Y	1002	5	14,14,15	0.81	1 (7%)	15,19,21	0.85	1 (6%)
6	HEM	Z	201	1,7	28,50,50	2.19	7 (25%)	17,82,82	1.78	6 (35%)
7	OXY	Z	202	6	1,1,1	0.27	0	0,0,0	0.00	-

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
6	HEM	1	201	2,7	-	0/6/54/54	0/0/8/8
7	OXY	1	202	6	-	0/0/0/0	0/0/0/0
8	NAG	2	1001	3	-	0/6/23/26	0/1/1/1
8	NAG	2	1002	8,3	-	0/6/23/26	0/1/1/1
8	NAG	2	1003	8	-	0/6/23/26	0/1/1/1
8	NAG	2	1004	8,3	-	0/6/23/26	0/1/1/1
8	NAG	2	1005	8	-	0/6/23/26	0/1/1/1
8	NAG	4	1001	5	-	0/6/23/26	0/1/1/1
8	NAG	4	1002	5	-	0/6/23/26	0/1/1/1
6	HEM	A	201	1,7	-	0/6/54/54	0/0/8/8
7	OXY	A	202	6	-	0/0/0/0	0/0/0/0
6	HEM	B	201	2,7	-	2/6/54/54	0/0/8/8
7	OXY	B	202	6	-	0/0/0/0	0/0/0/0
8	NAG	C	1001	3	-	0/6/23/26	0/1/1/1
8	NAG	C	1002	8,3	-	0/6/23/26	0/1/1/1
8	NAG	C	1003	8	-	0/6/23/26	0/1/1/1
8	NAG	C	1004	3	-	0/6/23/26	0/1/1/1
8	NAG	C	1005	8,3	-	0/6/23/26	0/1/1/1
8	NAG	C	1006	8	-	0/6/23/26	0/1/1/1
8	NAG	E	1001	5	-	0/6/23/26	0/1/1/1
8	NAG	E	1002	5	-	0/6/23/26	0/1/1/1
6	HEM	F	201	1,7	-	0/6/54/54	0/0/8/8
7	OXY	F	202	6	-	0/0/0/0	0/0/0/0
6	HEM	G	201	2,7	-	0/6/54/54	0/0/8/8
7	OXY	G	202	6	-	0/0/0/0	0/0/0/0
8	NAG	H	1001	3	-	0/6/23/26	0/1/1/1
8	NAG	H	1002	3	-	0/6/23/26	0/1/1/1
8	NAG	H	1003	8,3	-	0/6/23/26	0/1/1/1
8	NAG	H	1004	8	-	0/6/23/26	0/1/1/1
8	NAG	J	1001	5	-	0/6/23/26	0/1/1/1
8	NAG	J	1002	5	-	0/6/23/26	0/1/1/1
6	HEM	K	201	1,7	-	0/6/54/54	0/0/8/8
7	OXY	K	202	6	-	0/0/0/0	0/0/0/0
6	HEM	L	201	2,7	-	0/6/54/54	0/0/8/8
7	OXY	L	202	6	-	0/0/0/0	0/0/0/0
8	NAG	M	1001	3	-	0/6/23/26	0/1/1/1
8	NAG	M	1002	8,3	-	0/6/23/26	0/1/1/1
8	NAG	M	1003	8	-	0/6/23/26	0/1/1/1
8	NAG	M	1004	3	-	0/6/23/26	0/1/1/1
8	NAG	M	1005	8,3	-	0/6/23/26	0/1/1/1
8	NAG	M	1006	8	-	0/6/23/26	0/1/1/1
8	NAG	O	1001	5	-	0/6/23/26	0/1/1/1
8	NAG	O	1002	5	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	HEM	P	201	1,7	-	0/6/54/54	0/0/8/8
7	OXY	P	202	6	-	0/0/0/0	0/0/0/0
6	HEM	Q	201	2,7	-	0/6/54/54	0/0/8/8
7	OXY	Q	202	6	-	0/0/0/0	0/0/0/0
8	NAG	R	1001	3	-	0/6/23/26	0/1/1/1
8	NAG	R	1002	8,3	-	0/6/23/26	0/1/1/1
8	NAG	R	1003	8	-	0/6/23/26	0/1/1/1
8	NAG	R	1004	3	-	0/6/23/26	0/1/1/1
8	NAG	R	1005	8,3	-	0/6/23/26	0/1/1/1
8	NAG	R	1006	8	-	0/6/23/26	0/1/1/1
8	NAG	T	1001	5	-	0/6/23/26	0/1/1/1
8	NAG	T	1002	5	-	0/6/23/26	0/1/1/1
6	HEM	U	201	1,7	-	0/6/54/54	0/0/8/8
7	OXY	U	202	6	-	0/0/0/0	0/0/0/0
6	HEM	V	201	2,7	-	0/6/54/54	0/0/8/8
7	OXY	V	202	6	-	0/0/0/0	0/0/0/0
8	NAG	W	1001	3	-	0/6/23/26	0/1/1/1
8	NAG	W	1002	3	-	0/6/23/26	0/1/1/1
8	NAG	W	1003	8,3	-	0/6/23/26	0/1/1/1
8	NAG	W	1004	8	-	0/6/23/26	0/1/1/1
8	NAG	Y	1001	5	-	0/6/23/26	0/1/1/1
8	NAG	Y	1002	5	-	0/6/23/26	0/1/1/1
6	HEM	Z	201	1,7	-	0/6/54/54	0/0/8/8
7	OXY	Z	202	6	-	0/0/0/0	0/0/0/0

All (107) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	201	HEM	C3C-C2C	-6.91	1.31	1.40
6	1	201	HEM	C3B-C2B	-6.45	1.31	1.40
6	Q	201	HEM	C3C-C2C	-6.45	1.31	1.40
6	Q	201	HEM	C3B-C2B	-6.41	1.31	1.40
6	V	201	HEM	C3C-C2C	-6.20	1.32	1.40
6	1	201	HEM	C3C-C2C	-6.12	1.32	1.40
6	B	201	HEM	C3C-C2C	-6.01	1.32	1.40
6	K	201	HEM	C3B-C2B	-5.93	1.32	1.40
6	G	201	HEM	C3B-C2B	-5.89	1.32	1.40
6	L	201	HEM	C3B-C2B	-5.79	1.32	1.40
6	B	201	HEM	C3B-C2B	-5.74	1.32	1.40
6	L	201	HEM	C3C-C2C	-5.49	1.33	1.40
6	A	201	HEM	C3C-C2C	-4.86	1.33	1.40
6	V	201	HEM	C3B-C2B	-4.84	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	201	HEM	C3C-C2C	-4.63	1.34	1.40
6	K	201	HEM	C3C-C2C	-4.50	1.34	1.40
6	P	201	HEM	C3C-C2C	-4.29	1.34	1.40
6	Z	201	HEM	C3C-C2C	-4.23	1.34	1.40
6	U	201	HEM	C3C-C2C	-4.23	1.34	1.40
6	Z	201	HEM	C3B-C2B	-4.19	1.34	1.40
6	A	201	HEM	C3B-C2B	-3.93	1.35	1.40
6	U	201	HEM	C3B-C2B	-3.43	1.35	1.40
6	P	201	HEM	C3B-C2B	-3.41	1.35	1.40
8	O	1002	NAG	O5-C1	-3.38	1.38	1.43
6	F	201	HEM	C3B-C2B	-3.22	1.36	1.40
8	M	1001	NAG	O5-C1	-3.16	1.38	1.43
8	4	1002	NAG	O5-C1	-2.83	1.39	1.43
8	Y	1002	NAG	O5-C1	-2.69	1.39	1.43
8	R	1005	NAG	O5-C1	-2.47	1.39	1.43
8	E	1002	NAG	O5-C1	-2.45	1.39	1.43
8	J	1002	NAG	O5-C1	-2.36	1.39	1.43
8	T	1002	NAG	O5-C1	-2.04	1.40	1.43
6	B	201	HEM	C4B-CHC	-2.04	1.34	1.40
8	C	1003	NAG	C1-C2	2.01	1.55	1.52
6	Z	201	HEM	CAD-C3D	2.02	1.56	1.52
8	H	1001	NAG	O5-C1	2.07	1.47	1.43
6	Z	201	HEM	C4D-ND	2.09	1.39	1.36
6	L	201	HEM	CMD-C2D	2.11	1.55	1.51
8	W	1003	NAG	O5-C1	2.12	1.47	1.43
6	L	201	HEM	C1C-NC	2.15	1.39	1.36
6	1	201	HEM	C1C-NC	2.20	1.39	1.36
6	V	201	HEM	C1C-NC	2.22	1.39	1.36
8	R	1003	NAG	C1-C2	2.23	1.55	1.52
6	L	201	HEM	CAA-C2A	2.27	1.55	1.52
8	2	1003	NAG	C1-C2	2.29	1.55	1.52
6	G	201	HEM	C1C-NC	2.43	1.39	1.36
6	K	201	HEM	C4D-ND	2.44	1.39	1.36
6	Q	201	HEM	C4D-ND	2.44	1.39	1.36
6	P	201	HEM	CAA-C2A	2.54	1.56	1.52
6	F	201	HEM	CAA-C2A	2.57	1.56	1.52
8	2	1004	NAG	O5-C1	2.64	1.48	1.43
6	Q	201	HEM	C3C-CAC	2.67	1.53	1.47
6	K	201	HEM	CAA-C2A	2.68	1.56	1.52
6	G	201	HEM	CAA-C2A	2.70	1.56	1.52
6	1	201	HEM	CAA-C2A	2.71	1.56	1.52
6	G	201	HEM	C3C-CAC	2.72	1.53	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	201	HEM	C4D-ND	2.72	1.40	1.36
8	M	1003	NAG	C1-C2	2.77	1.56	1.52
6	V	201	HEM	C3C-CAC	2.82	1.53	1.47
6	A	201	HEM	C3C-CAC	2.85	1.53	1.47
6	L	201	HEM	C3C-CAC	2.90	1.53	1.47
6	Q	201	HEM	C3B-CAB	2.91	1.53	1.47
6	1	201	HEM	C3C-CAC	2.93	1.53	1.47
6	U	201	HEM	C4D-ND	2.93	1.40	1.36
6	K	201	HEM	C3C-CAC	2.96	1.53	1.47
6	B	201	HEM	C3C-CAC	2.98	1.53	1.47
6	1	201	HEM	C3B-CAB	2.98	1.53	1.47
6	P	201	HEM	C4D-ND	2.99	1.40	1.36
8	M	1005	NAG	C1-C2	3.03	1.56	1.52
6	B	201	HEM	C4D-ND	3.05	1.40	1.36
6	G	201	HEM	C3B-CAB	3.11	1.54	1.47
6	B	201	HEM	C3B-CAB	3.11	1.54	1.47
8	H	1003	NAG	O5-C1	3.19	1.48	1.43
6	F	201	HEM	C4D-ND	3.21	1.40	1.36
6	V	201	HEM	C3B-CAB	3.27	1.54	1.47
6	L	201	HEM	C4D-ND	3.28	1.40	1.36
6	K	201	HEM	C3B-CAB	3.29	1.54	1.47
8	M	1003	NAG	O5-C1	3.40	1.49	1.43
6	P	201	HEM	C3B-CAB	3.51	1.54	1.47
6	V	201	HEM	C4D-ND	3.59	1.41	1.36
6	L	201	HEM	C3B-CAB	3.61	1.55	1.47
8	C	1003	NAG	O5-C1	3.63	1.49	1.43
6	A	201	HEM	C3B-CAB	3.66	1.55	1.47
8	C	1004	NAG	O5-C1	3.68	1.49	1.43
6	P	201	HEM	C3C-CAC	3.78	1.55	1.47
8	C	1002	NAG	O5-C1	3.81	1.50	1.43
8	M	1004	NAG	O5-C1	3.82	1.50	1.43
6	U	201	HEM	C3C-CAC	3.87	1.55	1.47
6	Z	201	HEM	C3B-CAB	3.89	1.55	1.47
6	F	201	HEM	C3C-CAC	3.98	1.55	1.47
6	F	201	HEM	C3B-CAB	3.99	1.55	1.47
6	1	201	HEM	C4D-ND	4.02	1.41	1.36
6	Z	201	HEM	C3C-CAC	4.08	1.55	1.47
8	R	1003	NAG	O5-C1	4.10	1.50	1.43
6	U	201	HEM	C3B-CAB	4.52	1.56	1.47
6	K	201	HEM	C3D-C2D	4.89	1.52	1.37
6	B	201	HEM	C3D-C2D	5.09	1.52	1.37
6	G	201	HEM	C3D-C2D	5.14	1.52	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	201	HEM	C3D-C2D	5.25	1.53	1.37
6	Q	201	HEM	C3D-C2D	5.27	1.53	1.37
6	A	201	HEM	C3D-C2D	5.32	1.53	1.37
6	P	201	HEM	C3D-C2D	5.42	1.53	1.37
6	F	201	HEM	C3D-C2D	5.53	1.54	1.37
6	Z	201	HEM	C3D-C2D	5.57	1.54	1.37
6	1	201	HEM	C3D-C2D	5.64	1.54	1.37
6	U	201	HEM	C3D-C2D	5.68	1.54	1.37
6	V	201	HEM	C3D-C2D	6.01	1.55	1.37

All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Q	201	HEM	CAA-CBA-CGA	-5.98	102.45	112.66
6	L	201	HEM	CAD-CBD-CGD	-5.60	103.09	112.66
6	B	201	HEM	CAA-CBA-CGA	-5.48	103.30	112.66
6	B	201	HEM	CAD-CBD-CGD	-4.88	104.31	112.66
6	F	201	HEM	CMA-C3A-C4A	-4.63	121.36	128.46
6	L	201	HEM	CAA-CBA-CGA	-4.46	105.03	112.66
6	K	201	HEM	C1D-C2D-C3D	-4.40	103.93	107.00
6	K	201	HEM	CMA-C3A-C4A	-4.40	121.71	128.46
6	V	201	HEM	CAA-CBA-CGA	-3.89	106.02	112.66
6	G	201	HEM	CAA-CBA-CGA	-3.79	106.18	112.66
6	K	201	HEM	CBD-CAD-C3D	-3.78	105.25	112.47
6	L	201	HEM	CAA-C2A-C3A	-3.67	118.52	129.00
6	Q	201	HEM	CBD-CAD-C3D	-3.59	105.61	112.47
8	H	1003	NAG	C4-C3-C2	-3.53	105.84	111.02
6	B	201	HEM	CAA-C2A-C3A	-3.52	118.95	129.00
8	W	1003	NAG	C4-C3-C2	-3.35	106.10	111.02
8	C	1005	NAG	C4-C3-C2	-3.23	106.28	111.02
6	Z	201	HEM	C1D-C2D-C3D	-3.20	104.77	107.00
6	A	201	HEM	CMA-C3A-C4A	-3.10	123.70	128.46
8	M	1005	NAG	C4-C3-C2	-3.09	106.49	111.02
6	1	201	HEM	CAA-C2A-C3A	-3.03	120.34	129.00
6	1	201	HEM	CAA-CBA-CGA	-3.02	107.50	112.66
6	Q	201	HEM	CAD-CBD-CGD	-2.99	107.55	112.66
8	2	1004	NAG	C4-C3-C2	-2.98	106.66	111.02
6	Z	201	HEM	CAA-CBA-CGA	-2.94	107.64	112.66
6	A	201	HEM	C1D-C2D-C3D	-2.91	104.97	107.00
6	Q	201	HEM	C1D-C2D-C3D	-2.91	104.97	107.00
6	A	201	HEM	CAA-CBA-CGA	-2.89	107.73	112.66
6	P	201	HEM	CMA-C3A-C4A	-2.86	124.06	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Z	201	HEM	CBA-CAA-C2A	-2.79	107.15	112.48
6	G	201	HEM	C1D-C2D-C3D	-2.72	105.11	107.00
6	F	201	HEM	C1D-C2D-C3D	-2.70	105.12	107.00
6	L	201	HEM	CMA-C3A-C4A	-2.67	124.36	128.46
6	1	201	HEM	CAD-CBD-CGD	-2.62	108.19	112.66
6	K	201	HEM	CAD-CBD-CGD	-2.58	108.26	112.66
6	V	201	HEM	C1D-C2D-C3D	-2.55	105.22	107.00
6	P	201	HEM	CAA-CBA-CGA	-2.54	108.32	112.66
8	M	1001	NAG	C1-O5-C5	-2.51	108.71	112.17
6	L	201	HEM	CAD-C3D-C2D	-2.47	121.95	129.00
8	R	1005	NAG	O4-C4-C3	-2.40	105.13	110.36
6	U	201	HEM	CAA-CBA-CGA	-2.34	108.67	112.66
6	G	201	HEM	CAD-CBD-CGD	-2.34	108.67	112.66
6	G	201	HEM	CAA-C2A-C3A	-2.28	122.48	129.00
6	Q	201	HEM	CAA-C2A-C3A	-2.17	122.82	129.00
6	P	201	HEM	CAD-CBD-CGD	-2.09	109.10	112.66
6	A	201	HEM	CMC-C2C-C3C	2.03	128.66	124.89
8	Y	1002	NAG	C1-C2-N2	2.04	113.97	110.49
6	Z	201	HEM	CMC-C2C-C3C	2.08	128.76	124.89
6	A	201	HEM	CMD-C2D-C3D	2.09	128.89	124.94
8	C	1002	NAG	O4-C4-C5	2.12	114.61	109.28
6	Z	201	HEM	CMD-C2D-C3D	2.13	128.96	124.94
6	B	201	HEM	C4A-C3A-C2A	2.15	108.49	107.00
6	K	201	HEM	CMA-C3A-C2A	2.16	129.02	124.94
6	1	201	HEM	C4C-C3C-C2C	2.17	108.41	106.90
8	2	1004	NAG	C1-C2-N2	2.17	114.19	110.49
6	F	201	HEM	CMA-C3A-C2A	2.19	129.08	124.94
8	R	1005	NAG	C1-C2-N2	2.24	114.32	110.49
6	U	201	HEM	CMB-C2B-C3B	2.26	129.08	124.89
6	U	201	HEM	CMC-C2C-C3C	2.31	129.17	124.89
6	V	201	HEM	CMD-C2D-C3D	2.32	129.32	124.94
6	Z	201	HEM	C4A-C3A-C2A	2.33	108.62	107.00
8	R	1005	NAG	C3-C4-C5	2.38	114.41	110.22
6	L	201	HEM	CBA-CAA-C2A	2.39	117.05	112.48
6	K	201	HEM	CBA-CAA-C2A	2.45	117.18	112.48
8	W	1004	NAG	C1-O5-C5	2.47	115.56	112.17
8	H	1003	NAG	C1-C2-N2	2.51	114.77	110.49
8	C	1005	NAG	O4-C4-C3	2.51	115.81	110.36
8	M	1006	NAG	C1-O5-C5	2.51	115.63	112.17
8	W	1003	NAG	C1-C2-N2	2.51	114.78	110.49
6	Q	201	HEM	C4C-C3C-C2C	2.55	108.68	106.90
6	L	201	HEM	C4C-C3C-C2C	2.59	108.71	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	1005	NAG	C1-O5-C5	2.61	115.76	112.17
6	B	201	HEM	C4C-C3C-C2C	2.62	108.73	106.90
8	H	1004	NAG	C1-O5-C5	2.62	115.78	112.17
8	M	1005	NAG	O4-C4-C5	2.63	115.91	109.28
8	R	1006	NAG	C2-N2-C7	2.70	126.88	122.94
8	W	1003	NAG	O4-C4-C3	2.72	116.27	110.36
8	C	1005	NAG	C1-C2-N2	2.76	115.20	110.49
8	2	1004	NAG	O4-C4-C3	2.76	116.37	110.36
6	G	201	HEM	CBA-CAA-C2A	2.84	117.92	112.48
8	M	1005	NAG	O4-C4-C3	2.86	116.59	110.36
6	1	201	HEM	CBA-CAA-C2A	2.87	117.97	112.48
6	G	201	HEM	C4A-C3A-C2A	2.88	109.00	107.00
8	H	1003	NAG	O4-C4-C3	2.92	116.70	110.36
8	2	1005	NAG	C1-O5-C5	2.99	116.28	112.17
8	M	1005	NAG	C1-C2-N2	2.99	115.60	110.49
8	2	1003	NAG	C1-O5-C5	3.03	116.34	112.17
6	G	201	HEM	C4C-C3C-C2C	3.09	109.06	106.90
8	M	1004	NAG	C1-O5-C5	3.28	116.68	112.17
6	K	201	HEM	C4A-C3A-C2A	3.28	109.28	107.00
8	E	1002	NAG	C2-N2-C7	3.36	127.84	122.94
8	W	1003	NAG	O4-C4-C5	3.36	117.75	109.28
8	2	1004	NAG	O4-C4-C5	3.40	117.86	109.28
6	L	201	HEM	C4A-C3A-C2A	3.40	109.36	107.00
8	C	1004	NAG	C1-O5-C5	3.60	117.13	112.17
8	T	1002	NAG	C2-N2-C7	3.62	128.22	122.94
8	H	1003	NAG	O4-C4-C5	3.63	118.44	109.28
8	C	1005	NAG	O4-C4-C5	3.65	118.49	109.28
6	F	201	HEM	C4A-C3A-C2A	3.69	109.56	107.00
8	2	1002	NAG	C1-O5-C5	3.80	117.41	112.17
8	M	1003	NAG	C1-O5-C5	3.86	117.49	112.17
6	P	201	HEM	C4A-C3A-C2A	3.89	109.70	107.00
6	1	201	HEM	C4A-C3A-C2A	3.92	109.72	107.00
8	2	1004	NAG	C1-O5-C5	3.98	117.65	112.17
8	R	1003	NAG	C1-O5-C5	4.01	117.69	112.17
8	C	1003	NAG	C1-O5-C5	4.07	117.78	112.17
8	W	1002	NAG	C1-O5-C5	4.33	118.13	112.17
8	R	1005	NAG	C1-O5-C5	4.50	118.37	112.17
8	W	1003	NAG	C1-O5-C5	4.51	118.39	112.17
8	H	1003	NAG	C1-O5-C5	4.55	118.43	112.17
8	R	1002	NAG	C1-O5-C5	5.02	119.09	112.17
8	C	1005	NAG	C1-O5-C5	5.08	119.17	112.17
8	C	1002	NAG	C1-O5-C5	5.73	120.06	112.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	M	1002	NAG	C1-O5-C5	7.18	122.06	112.17

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	201	HEM	C3A-C2A-CAA-CBA
6	B	201	HEM	C1A-C2A-CAA-CBA

There are no ring outliers.

38 monomers are involved in 69 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	1	201	HEM	6	0
8	2	1002	NAG	2	0
8	2	1004	NAG	1	0
8	4	1002	NAG	2	0
6	A	201	HEM	1	0
6	B	201	HEM	6	0
8	C	1002	NAG	1	0
8	C	1003	NAG	1	0
8	C	1005	NAG	1	0
8	C	1006	NAG	1	0
8	E	1002	NAG	1	0
6	F	201	HEM	2	0
6	G	201	HEM	3	0
8	H	1003	NAG	1	0
8	H	1004	NAG	2	0
8	J	1002	NAG	2	0
6	K	201	HEM	1	0
6	L	201	HEM	6	0
8	M	1001	NAG	1	0
8	M	1002	NAG	1	0
8	M	1005	NAG	1	0
8	M	1006	NAG	1	0
8	O	1002	NAG	1	0
6	P	201	HEM	2	0
6	Q	201	HEM	4	0
8	R	1002	NAG	2	0
8	R	1003	NAG	1	0
8	R	1006	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	T	1002	NAG	1	0
6	U	201	HEM	4	0
7	U	202	OXY	1	0
6	V	201	HEM	3	0
7	V	202	OXY	1	0
8	W	1002	NAG	1	0
8	W	1003	NAG	1	0
8	Y	1002	NAG	1	0
6	Z	201	HEM	2	0
7	Z	202	OXY	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	A	141/141 (100%)	-0.38	0 100 100	40, 52, 72, 81	0
1	F	141/141 (100%)	-0.36	0 100 100	49, 67, 83, 92	0
1	K	141/141 (100%)	-0.39	0 100 100	37, 53, 76, 86	0
1	P	141/141 (100%)	-0.40	0 100 100	53, 67, 91, 107	0
1	U	141/141 (100%)	-0.30	0 100 100	59, 76, 98, 100	0
1	Z	141/141 (100%)	-0.38	0 100 100	58, 72, 89, 93	0
2	1	146/146 (100%)	-0.41	1 (0%) 87 75	67, 79, 104, 138	0
2	B	146/146 (100%)	-0.38	0 100 100	39, 60, 90, 117	0
2	G	146/146 (100%)	-0.32	2 (1%) 75 57	50, 66, 97, 118	0
2	L	146/146 (100%)	-0.39	0 100 100	39, 62, 94, 120	0
2	Q	146/146 (100%)	-0.35	0 100 100	53, 69, 102, 133	0
2	V	146/146 (100%)	-0.37	0 100 100	66, 78, 105, 137	0
3	2	310/315 (98%)	-0.20	1 (0%) 93 86	63, 80, 96, 115	0
3	C	310/315 (98%)	-0.27	1 (0%) 93 86	38, 57, 75, 93	0
3	H	310/315 (98%)	-0.19	2 (0%) 89 77	56, 74, 94, 114	0
3	M	310/315 (98%)	-0.24	1 (0%) 93 86	38, 55, 79, 96	0
3	R	310/315 (98%)	-0.20	1 (0%) 93 86	65, 79, 100, 107	0
3	W	310/315 (98%)	-0.08	2 (0%) 89 77	76, 92, 112, 121	0
4	3	144/146 (98%)	-0.34	2 (1%) 75 57	60, 75, 95, 115	0
4	D	144/146 (98%)	-0.38	2 (1%) 75 57	51, 65, 84, 101	0
4	I	144/146 (98%)	-0.34	0 100 100	49, 72, 95, 111	0
4	N	144/146 (98%)	-0.30	2 (1%) 75 57	54, 68, 88, 100	0
4	S	144/146 (98%)	-0.34	0 100 100	53, 74, 94, 109	0
4	X	144/146 (98%)	-0.35	1 (0%) 87 75	61, 78, 100, 115	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
5	4	261/343 (76%)	-0.02	18 (6%)	18 7	74, 102, 153, 172	2 (0%)
5	E	261/343 (76%)	-0.06	13 (4%)	30 13	42, 82, 146, 155	2 (0%)
5	J	261/343 (76%)	0.24	23 (8%)	11 4	68, 110, 203, 212	2 (0%)
5	O	261/343 (76%)	-0.08	14 (5%)	26 12	43, 83, 140, 151	2 (0%)
5	T	261/343 (76%)	0.23	24 (9%)	10 3	68, 111, 197, 212	2 (0%)
5	Y	261/343 (76%)	0.26	28 (10%)	7 2	82, 111, 205, 213	2 (0%)
All	All	6012/6546 (91%)	-0.19	138 (2%)	61 39	37, 76, 138, 213	12 (0%)

All (138) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	T	293	ALA	8.8
5	T	294	GLN	7.9
5	J	118	ALA	7.6
5	J	296	GLU	7.3
5	J	219	ASN	7.2
5	Y	294	GLN	7.2
5	Y	293	ALA	7.1
5	T	219	ASN	7.0
5	T	296	GLU	6.3
5	T	118	ALA	6.2
5	E	219	ASN	6.1
5	Y	118	ALA	6.0
5	Y	296	GLU	5.9
5	J	293	ALA	5.6
5	T	115	ASP	5.5
5	4	294	GLN	5.1
5	J	294	GLN	5.0
5	4	114	ASN	5.0
5	T	106	ARG	4.9
5	J	289	HIS	4.8
5	J	115	ASP	4.8
5	T	38	GLY	4.8
5	O	219	ASN	4.7
5	T	291	THR	4.6
5	J	290	GLU	4.6
5	Y	291	THR	4.5
5	Y	290	GLU	4.4
5	Y	117	LYS	4.4
5	Y	114	ASN	4.3

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Mol	Chain	Res	Type	RSRZ
5	Y	115	ASP	4.1
5	4	185	ASN	4.1
4	3	228	SER	4.1
5	E	112	LYS	4.1
5	Y	289	HIS	4.1
5	Y	219	ASN	4.0
5	4	291	THR	4.0
5	Y	295	GLU	4.0
5	T	185	ASN	3.9
5	E	114	ASN	3.8
5	E	294	GLN	3.8
5	O	114	ASN	3.8
5	J	195	GLU	3.7
5	4	219	ASN	3.6
5	Y	185	ASN	3.5
4	X	229	LEU	3.5
5	J	106	ARG	3.5
5	J	114	ASN	3.5
5	T	114	ASN	3.4
5	Y	106	ARG	3.4
5	Y	105	GLN	3.4
5	J	185	ASN	3.4
5	O	185	ASN	3.3
5	T	295	GLU	3.3
5	J	295	GLU	3.3
5	J	291	THR	3.3
5	4	189	ASP	3.3
5	4	112	LYS	3.2
5	4	220	VAL	3.2
5	O	294	GLN	3.2
5	Y	109	GLU	3.2
4	D	229	LEU	3.1
5	J	38	GLY	3.1
5	T	111	GLY	3.1
3	2	93	PRO	3.1
5	O	291	THR	3.1
5	T	195	GLU	3.1
5	T	290	GLU	3.1
5	4	195	GLU	3.1
5	Y	189	ASP	3.0
5	T	105	GLN	3.0
3	H	93	PRO	3.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
5	Y	191	LYS	3.0
5	O	184	GLY	2.9
5	Y	38	GLY	2.9
5	J	105	GLN	2.8
4	N	229	LEU	2.8
3	C	93	PRO	2.8
5	T	289	HIS	2.8
5	4	183	LYS	2.8
4	N	228	SER	2.8
5	Y	110	LEU	2.7
5	E	38	GLY	2.7
5	J	117	LYS	2.7
3	W	353	SER	2.7
5	E	185	ASN	2.6
5	Y	113	ALA	2.6
5	E	191	LYS	2.6
2	G	146	HIS	2.6
5	E	290	GLU	2.6
5	O	38	GLY	2.6
5	E	227	LYS	2.5
5	E	184	GLY	2.5
5	O	284	GLU	2.5
5	J	36	ALA	2.5
5	T	112	LYS	2.4
5	Y	36	ALA	2.4
3	H	157	ASN	2.4
5	E	41	THR	2.4
5	E	183	LYS	2.4
5	O	183	LYS	2.4
3	M	93	PRO	2.4
5	T	286	LYS	2.4
5	4	116	THR	2.4
5	J	186	GLY	2.3
5	T	191	LYS	2.3
5	Y	286	LYS	2.3
4	3	229	LEU	2.3
3	R	93	PRO	2.3
5	O	290	GLU	2.3
2	1	2	HIS	2.3
5	O	196	LYS	2.2
3	W	93	PRO	2.2
4	D	178	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
5	T	186	GLY	2.2
5	J	286	LYS	2.2
5	4	184	GLY	2.2
5	J	111	GLY	2.2
5	E	284	GLU	2.2
5	4	186	GLY	2.2
5	Y	269	LYS	2.2
5	O	41	THR	2.1
5	T	183	LYS	2.1
5	4	36	ALA	2.1
5	O	191	LYS	2.1
5	T	117	LYS	2.1
2	G	2	HIS	2.1
5	J	183	LYS	2.1
5	Y	217	ALA	2.1
5	4	290	GLU	2.1
5	T	109	GLU	2.1
5	4	38	GLY	2.1
5	Y	112	LYS	2.0
5	O	186	GLY	2.0
5	4	191	LYS	2.0
5	Y	187	SER	2.0
5	4	218	ALA	2.0
5	Y	186	GLY	2.0
5	J	287	ASN	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 carbohydrates in this entry.

## 6.4 Ligands ⓘ

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( $\text{\AA}^2$ )	Q<0.9
6	HEM	1	201	43/43	0.95	0.24	1.28	63,68,73,76	0
6	HEM	B	201	43/43	0.96	0.23	0.57	41,50,60,64	0
8	NAG	Y	1002	14/15	0.84	0.22	0.40	81,85,88,90	0
6	HEM	A	201	43/43	0.95	0.21	0.35	51,55,60,62	0
6	HEM	V	201	43/43	0.96	0.21	0.24	65,69,74,76	0
6	HEM	Z	201	43/43	0.95	0.21	0.24	63,71,79,82	0
6	HEM	U	201	43/43	0.95	0.23	0.22	68,78,88,92	0
6	HEM	F	201	43/43	0.94	0.23	0.21	56,65,76,80	0
6	HEM	Q	201	43/43	0.95	0.23	0.20	58,60,62,63	0
6	HEM	G	201	43/43	0.95	0.22	0.14	53,58,64,67	0
6	HEM	P	201	43/43	0.95	0.22	0.14	63,71,79,83	0
6	HEM	K	201	43/43	0.94	0.21	0.08	43,57,69,73	0
8	NAG	2	1004	14/15	0.89	0.22	-0.09	97,97,97,97	0
6	HEM	L	201	43/43	0.95	0.21	-0.12	45,50,57,59	0
8	NAG	H	1003	14/15	0.85	0.23	-0.13	89,89,89,89	0
8	NAG	J	1002	14/15	0.89	0.17	-0.14	80,83,86,87	0
8	NAG	4	1002	14/15	0.91	0.19	-0.16	81,83,86,87	0
8	NAG	M	1005	14/15	0.84	0.21	-0.46	75,75,75,75	0
8	NAG	R	1005	14/15	0.87	0.20	-0.47	88,88,88,88	0
8	NAG	C	1005	14/15	0.87	0.18	-0.62	77,77,77,77	0
8	NAG	W	1003	14/15	0.85	0.22	-0.72	107,107,107,107	0
8	NAG	M	1006	14/15	0.81	0.22	-0.78	86,86,86,86	0
8	NAG	O	1002	14/15	0.88	0.17	-0.86	60,65,68,70	0
8	NAG	R	1006	14/15	0.79	0.22	-0.95	94,94,94,94	0
8	NAG	2	1005	14/15	0.81	0.18	-1.02	106,106,106,106	0
8	NAG	C	1006	14/15	0.83	0.17	-1.26	89,89,89,89	0
8	NAG	E	1002	14/15	0.92	0.14	-1.45	63,67,70,70	0
8	NAG	W	1004	14/15	0.74	0.23	-1.56	116,116,116,116	0
8	NAG	T	1002	14/15	0.93	0.11	-1.61	76,80,86,86	0
8	NAG	E	1001	14/15	0.85	0.42	-	103,107,112,113	0
8	NAG	H	1001	14/15	0.90	0.36	-	81,81,81,81	0
8	NAG	R	1002	14/15	0.69	0.33	-	105,105,105,105	0
8	NAG	J	1001	14/15	0.76	0.50	-	136,144,151,154	0
8	NAG	2	1001	14/15	0.87	0.37	-	101,101,101,101	0
8	NAG	H	1002	14/15	0.76	0.26	-	85,85,85,85	0
7	OXY	K	202	2/2	0.96	0.23	-	62,62,62,64	0
8	NAG	W	1001	14/15	0.88	0.39	-	101,101,101,101	0
7	OXY	A	202	2/2	0.94	0.30	-	61,61,61,62	0
7	OXY	1	202	2/2	0.99	0.21	-	69,69,69,69	0
8	NAG	C	1001	14/15	0.79	0.42	-	84,84,84,84	0
8	NAG	R	1004	14/15	0.49	0.49	-	123,123,123,123	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
7	OXY	F	202	2/2	0.97	0.29	-	72,72,72,72	0
8	NAG	M	1001	14/15	0.83	0.40	-	92,92,92,92	0
7	OXY	U	202	2/2	0.95	0.25	-	80,80,80,81	0
8	NAG	R	1001	14/15	0.83	0.38	-	94,94,94,94	0
8	NAG	4	1001	14/15	0.80	0.45	-	125,128,131,132	0
8	NAG	R	1003	14/15	0.83	0.37	-	112,112,112,112	0
7	OXY	Z	202	2/2	0.96	0.18	-	75,75,75,76	0
8	NAG	Y	1001	14/15	0.82	0.39	-	133,142,147,151	0
7	OXY	V	202	2/2	0.98	0.17	-	69,69,69,69	0
8	NAG	M	1004	14/15	0.70	0.44	-	116,116,116,116	0
7	OXY	Q	202	2/2	0.93	0.31	-	62,62,62,63	0
8	NAG	C	1003	14/15	0.89	0.31	-	94,94,94,94	0
8	NAG	2	1002	14/15	0.71	0.37	-	118,118,118,118	0
8	NAG	H	1004	14/15	0.79	0.22	-	98,98,98,98	0
8	NAG	O	1001	14/15	0.80	0.40	-	101,107,112,116	0
7	OXY	L	202	2/2	0.98	0.19	-	47,47,47,47	0
8	NAG	W	1002	14/15	0.66	0.34	-	112,112,112,112	0
8	NAG	C	1004	14/15	0.71	0.48	-	112,112,112,112	0
7	OXY	P	202	2/2	0.98	0.24	-	70,70,70,72	0
7	OXY	G	202	2/2	0.96	0.28	-	59,59,59,60	0
8	NAG	M	1002	14/15	0.71	0.32	-	90,90,90,90	0
8	NAG	T	1001	14/15	0.73	0.51	-	143,148,153,154	0
8	NAG	M	1003	14/15	0.80	0.40	-	97,97,97,97	0
8	NAG	C	1002	14/15	0.78	0.30	-	86,86,86,86	0
8	NAG	2	1003	14/15	0.83	0.37	-	123,123,123,123	0
7	OXY	B	202	2/2	0.97	0.22	-	49,49,49,51	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.