



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2023 – 01:08 PM EDT

PDB ID : 3GYR  
Title : Structure of Phenoxazinone synthase from *Streptomyces antibioticus* reveals a new type 2 copper center.  
Authors : Smith, A.W.; Camara-Artigas, A.; Wang, M.; Francisco, W.A.; Allen, J.P.  
Deposited on : 2009-04-05  
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35

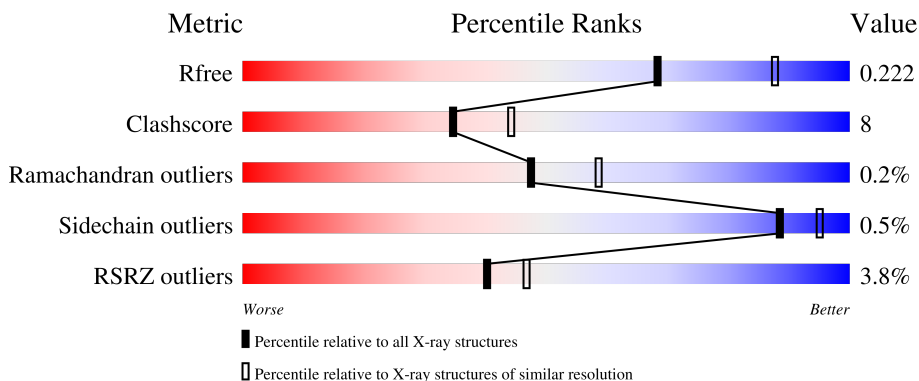
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 Å.

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



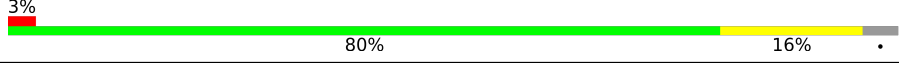
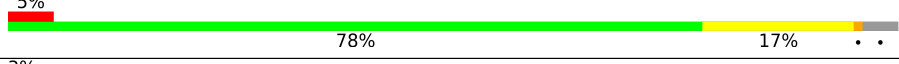

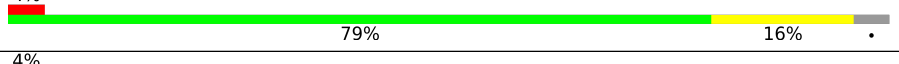
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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

Mol	Chain	Length	Quality of chain
1	A	612	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 78%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 17%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">5%      78%      17%      . .</p>
1	B	612	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 83%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">3%      83%      13%      .</p>
1	C	612	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 85%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">3%      85%      11%      . .</p>
1	D	612	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 82%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 3%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">2%      82%      13%      .</p>
1	E	612	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 84%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 4%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">4%      84%      12%      .</p>

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	612	 4% 81% 14% . .
1	G	612	 4% 82% 13% . .
1	H	612	 3% 80% 16% .
1	I	612	 5% 78% 17% . .
1	J	612	 3% 81% 15% . .
1	K	612	 4% 79% 16% .
1	L	612	 4% 80% 15% . .

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 59241 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 Phenoxazinone synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	587	4560	2886	812	847	15	0	0	0
1	B	587	4560	2886	812	847	15	0	0	0
1	C	587	4560	2886	812	847	15	0	0	0
1	D	587	4560	2886	812	847	15	0	0	0
1	E	587	4560	2886	812	847	15	0	0	0
1	F	587	4560	2886	812	847	15	0	0	0
1	G	587	4560	2886	812	847	15	0	0	0
1	H	587	4560	2886	812	847	15	0	0	0
1	I	587	4560	2886	812	847	15	0	0	0
1	J	587	4560	2886	812	847	15	0	0	0
1	K	587	4560	2886	812	847	15	0	0	0
1	L	587	4560	2886	812	847	15	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	496	ARG	ALA	engineered mutation	UNP Q53692
B	496	ARG	ALA	engineered mutation	UNP Q53692
C	496	ARG	ALA	engineered mutation	UNP Q53692
D	496	ARG	ALA	engineered mutation	UNP Q53692
E	496	ARG	ALA	engineered mutation	UNP Q53692

*Continued on next page...*

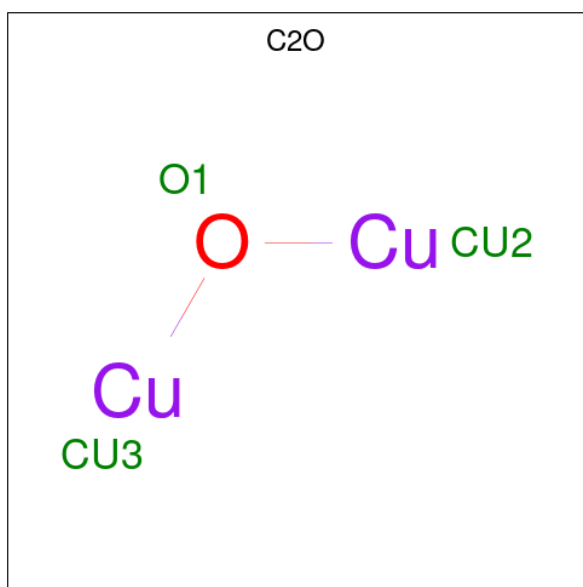
*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
F	496	ARG	ALA	engineered mutation	UNP Q53692
G	496	ARG	ALA	engineered mutation	UNP Q53692
H	496	ARG	ALA	engineered mutation	UNP Q53692
I	496	ARG	ALA	engineered mutation	UNP Q53692
J	496	ARG	ALA	engineered mutation	UNP Q53692
K	496	ARG	ALA	engineered mutation	UNP Q53692
L	496	ARG	ALA	engineered mutation	UNP Q53692

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	3	Total Cu 3 3	0	0
2	B	3	Total Cu 3 3	0	0
2	C	3	Total Cu 3 3	0	0
2	D	3	Total Cu 3 3	0	0
2	E	3	Total Cu 3 3	0	0
2	F	3	Total Cu 3 3	0	0
2	G	3	Total Cu 3 3	0	0
2	H	3	Total Cu 3 3	0	0
2	I	3	Total Cu 3 3	0	0
2	J	3	Total Cu 3 3	0	0
2	K	3	Total Cu 3 3	0	0
2	L	3	Total Cu 3 3	0	0

- Molecule 3 is CU-O-CU LINKAGE (three-letter code: C2O) (formula: Cu<sub>2</sub>O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Cu	O		
3	A	1	3	2	1	0	0
3	B	1	3	2	1	0	0
3	C	1	3	2	1	0	0
3	D	1	3	2	1	0	0
3	E	1	3	2	1	0	0
3	F	1	3	2	1	0	0
3	G	1	3	2	1	0	0
3	H	1	3	2	1	0	0
3	I	1	3	2	1	0	0
3	J	1	3	2	1	0	0
3	K	1	3	2	1	0	0
3	L	1	3	2	1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	D	1	Total C O 6 3 3	0	0
4	E	1	Total C O 6 3 3	0	0
4	F	1	Total C O 6 3 3	0	0
4	G	1	Total C O 6 3 3	0	0
4	H	1	Total C O 6 3 3	0	0
4	I	1	Total C O 6 3 3	0	0
4	J	1	Total C O 6 3 3	0	0
4	K	1	Total C O 6 3 3	0	0
4	L	1	Total C O 6 3 3	0	0

- Molecule 5 is water.

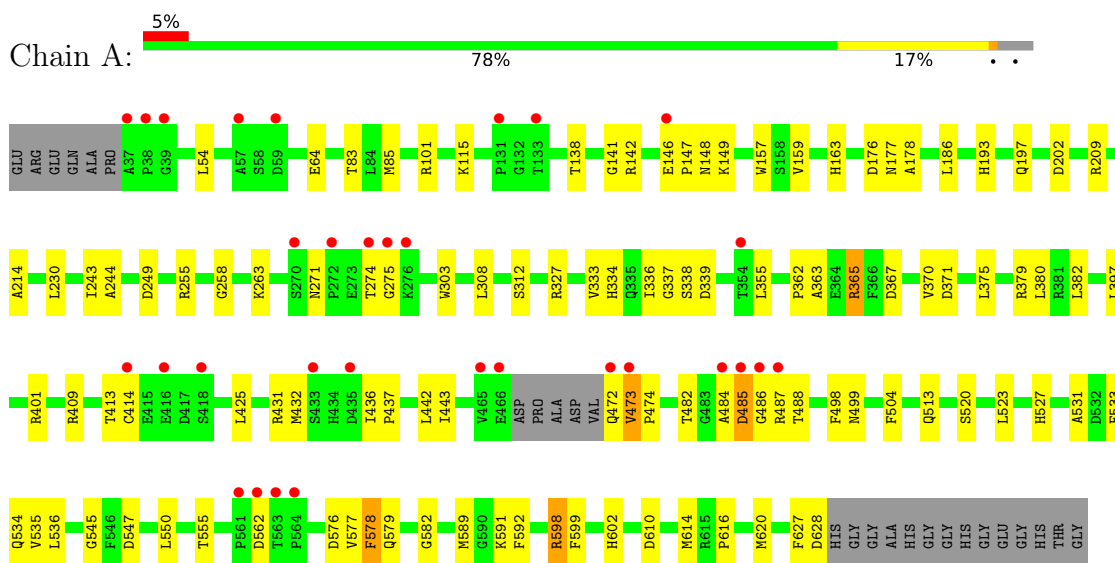
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	354	Total 354	O 354	0	0
5	B	362	Total 362	O 362	0	0
5	C	398	Total 398	O 398	0	0
5	D	386	Total 386	O 386	0	0
5	E	357	Total 357	O 357	0	0
5	F	361	Total 361	O 361	0	0
5	G	359	Total 359	O 359	0	0
5	H	376	Total 376	O 376	0	0
5	I	330	Total 330	O 330	0	0
5	J	388	Total 388	O 388	0	0
5	K	359	Total 359	O 359	0	0
5	L	347	Total 347	O 347	0	0



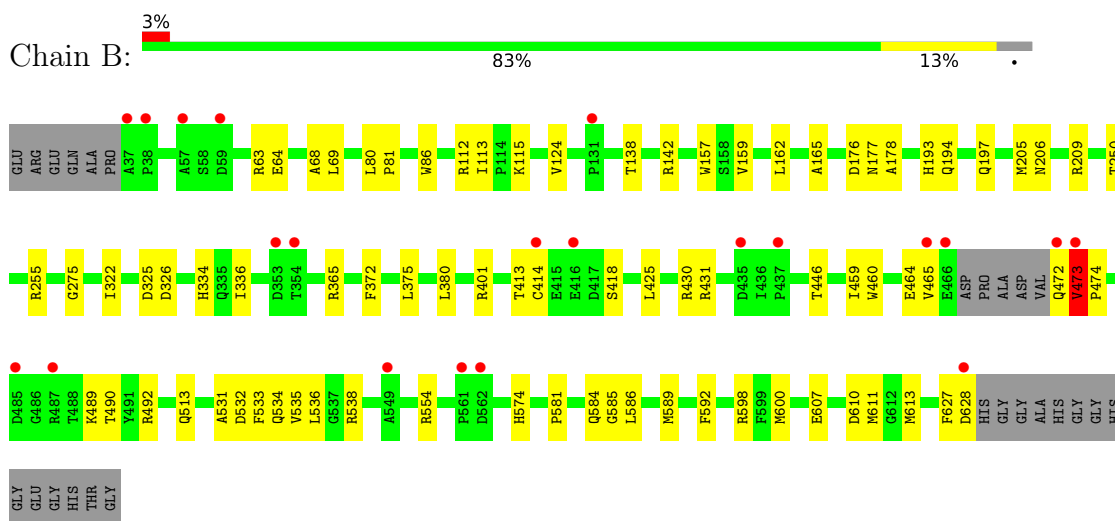
### 3 Residue-property plots

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

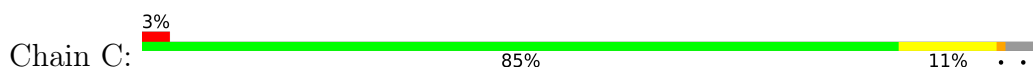
- Molecule 1: Phenoxazinone synthase

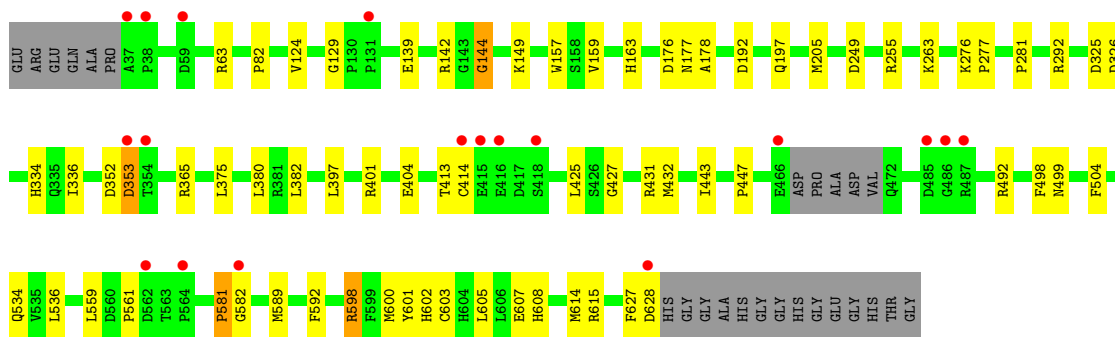


- Molecule 1: Phenoxazinone synthase

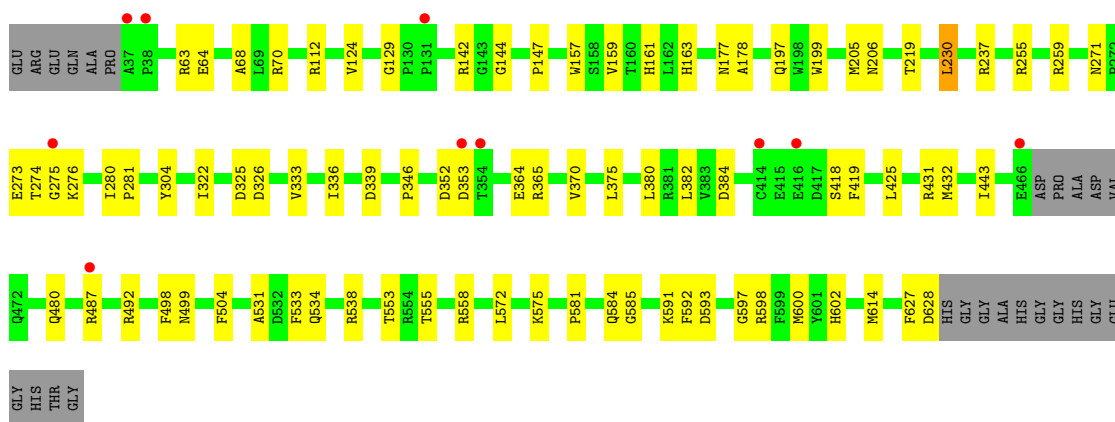
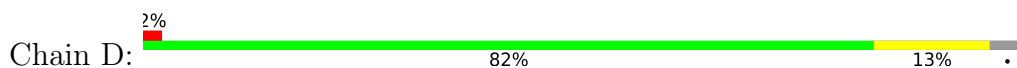


- Molecule 1: Phenoxazinone synthase

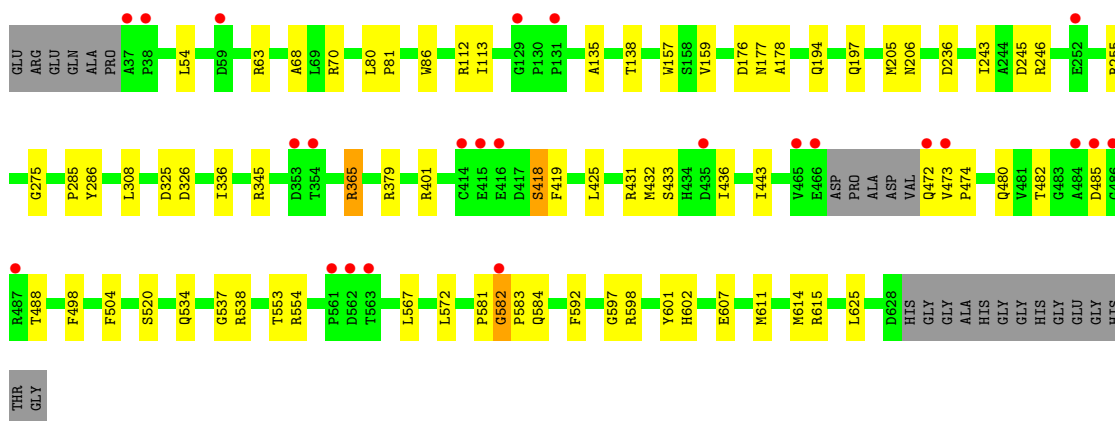
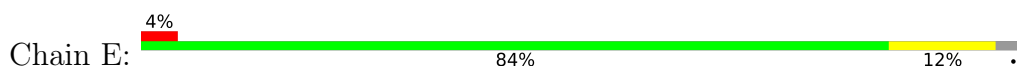




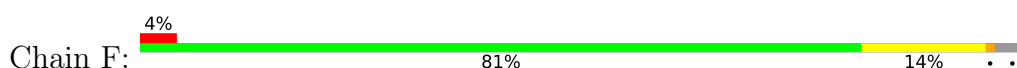
• Molecule 1: Phenoxazinone synthase

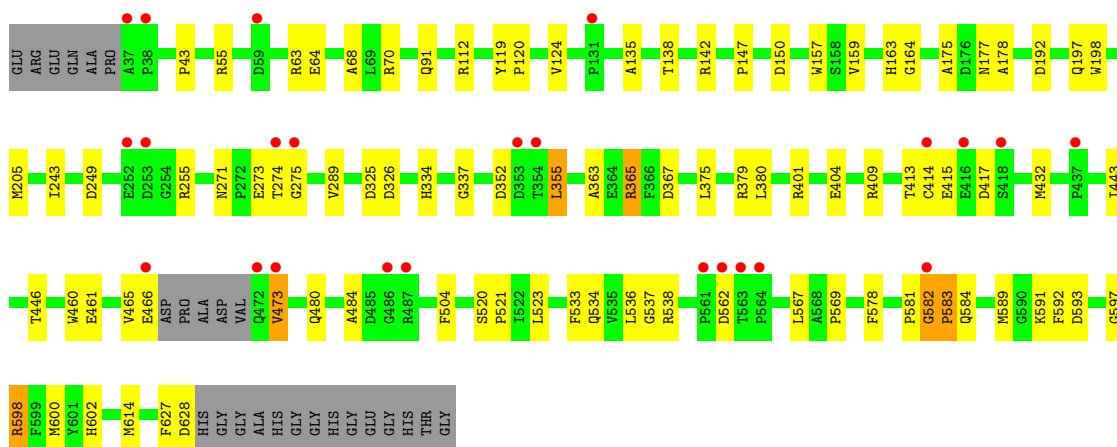


• Molecule 1: Phenoxazinone synthase

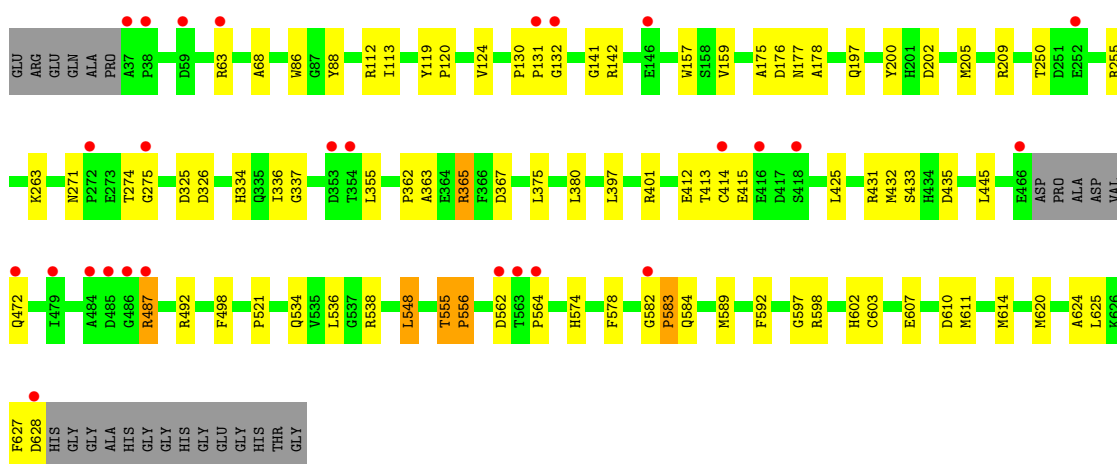
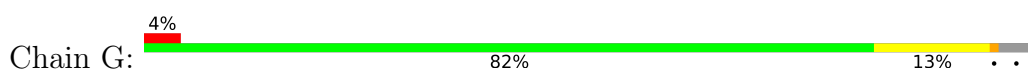


• Molecule 1: Phenoxazinone synthase

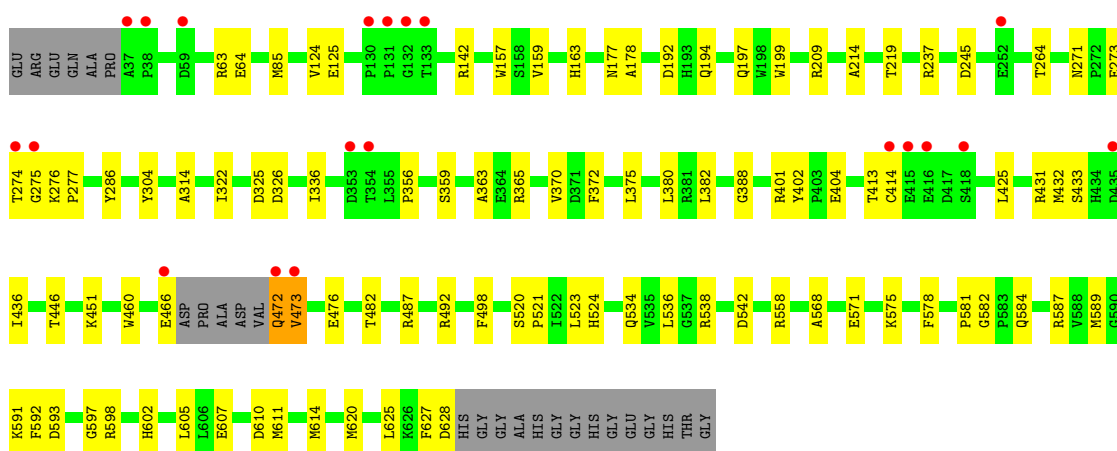
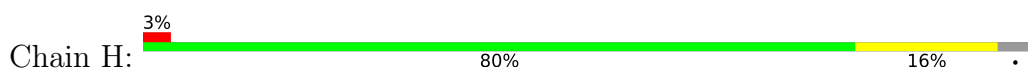




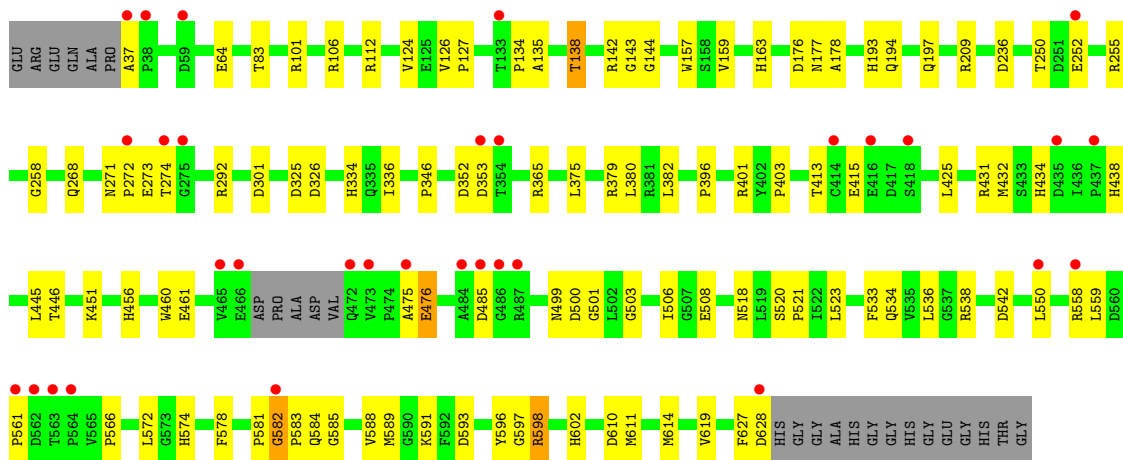
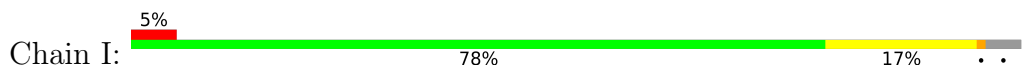
• Molecule 1: Phenoxazinone synthase



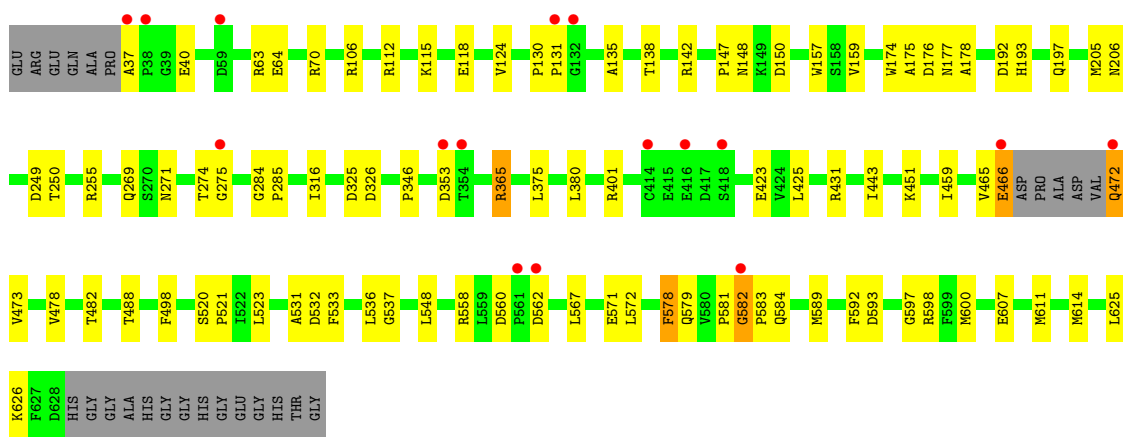
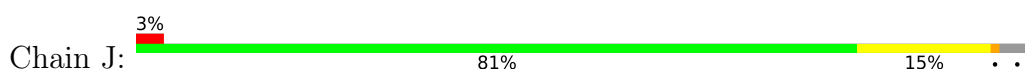
• Molecule 1: Phenoxazinone synthase



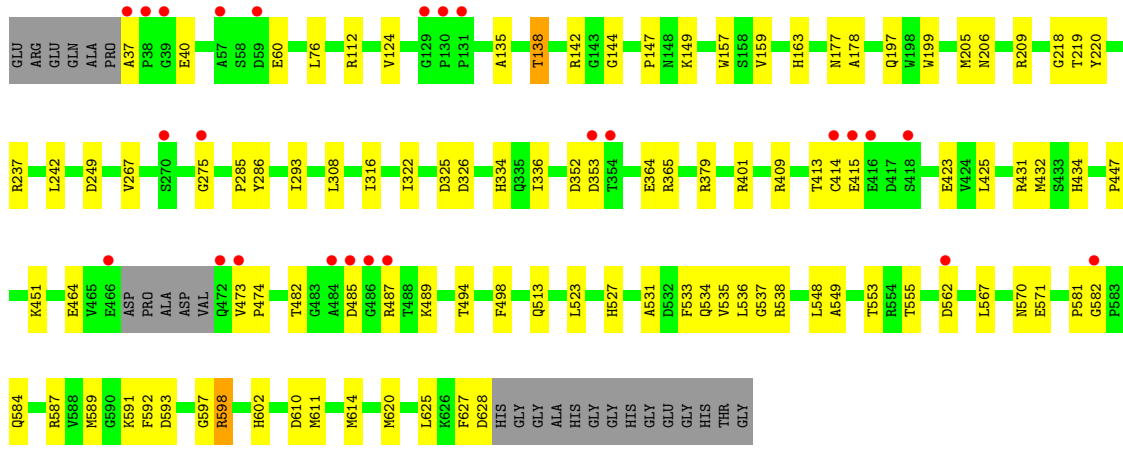
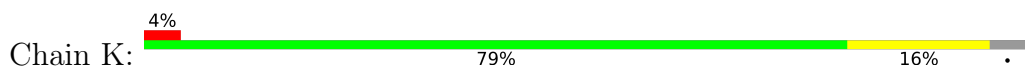
• Molecule 1: Phenoxazinone synthase



• Molecule 1: Phenoxazinone synthase

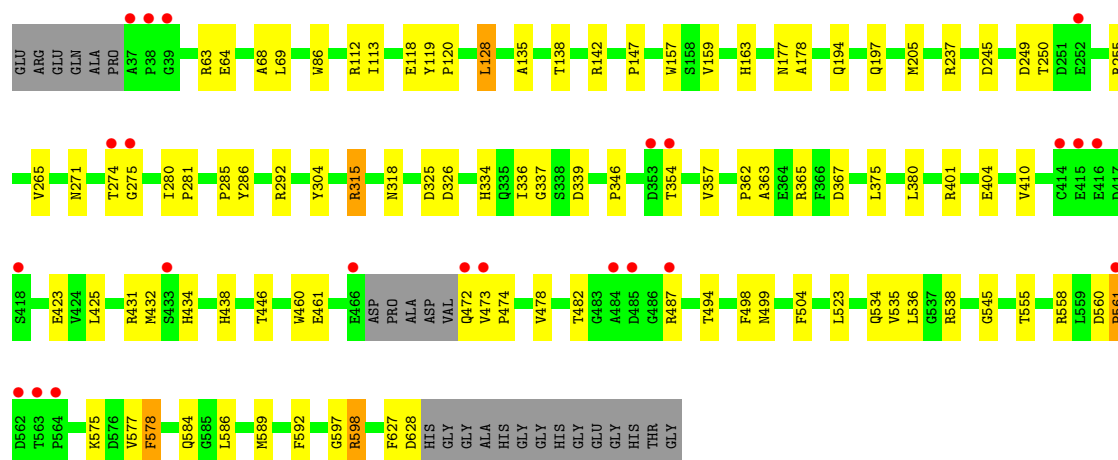


• Molecule 1: Phenoxazinone synthase



- Molecule 1: Phenoxazinone synthase

Chain L: 4% 80% 15%



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	109.49Å 163.46Å 164.35Å 117.04° 95.74° 107.23°	Depositor
Resolution (Å)	20.00 – 2.30 20.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	86.3 (20.00-2.30) 86.3 (20.00-2.30)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.54 (at 2.30Å)	Xtrriage
Refinement program	REFMAC 5.5.0072, CNS	Depositor
R, $R_{free}$	0.165 , 0.222 0.165 , 0.222	Depositor DCC
$R_{free}$ test set	17920 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.2	Xtrriage
Anisotropy	0.053	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 53.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.007 for -h,h+k+1,-l	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	59241	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CU, C2O

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	0.66	0/4697	0.75	4/6423 (0.1%)
1	B	0.65	0/4697	0.74	0/6423
1	C	0.68	1/4697 (0.0%)	0.76	2/6423 (0.0%)
1	D	0.67	0/4697	0.73	2/6423 (0.0%)
1	E	0.67	0/4697	0.74	2/6423 (0.0%)
1	F	0.67	0/4697	0.74	3/6423 (0.0%)
1	G	0.69	1/4697 (0.0%)	0.76	2/6423 (0.0%)
1	H	0.66	0/4697	0.74	2/6423 (0.0%)
1	I	0.67	0/4697	0.74	3/6423 (0.0%)
1	J	0.67	0/4697	0.75	5/6423 (0.1%)
1	K	0.66	0/4697	0.74	2/6423 (0.0%)
1	L	0.65	0/4697	0.74	3/6423 (0.0%)
All	All	0.67	2/56364 (0.0%)	0.74	30/77076 (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
1	A	0	2
1	B	0	4
1	C	0	5
1	D	0	5
1	E	0	2
1	F	0	4
1	G	0	2
1	H	0	2
1	I	0	1
1	J	0	3
1	K	0	5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	2
All	All	0	37

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	603	CYS	CB-SG	-6.39	1.71	1.82
1	C	603	CYS	CB-SG	-5.81	1.72	1.81

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	365	ARG	NE-CZ-NH2	-9.62	115.49	120.30
1	A	365	ARG	NE-CZ-NH1	6.75	123.68	120.30
1	I	292	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	A	598	ARG	NE-CZ-NH2	-6.15	117.22	120.30
1	C	292	ARG	NE-CZ-NH1	5.97	123.29	120.30
1	G	548	LEU	CA-CB-CG	5.82	128.68	115.30
1	I	292	ARG	NE-CZ-NH2	-5.81	117.40	120.30
1	K	598	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	C	598	ARG	NE-CZ-NH2	-5.57	117.51	120.30
1	F	365	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	I	598	ARG	NE-CZ-NH2	-5.51	117.54	120.30
1	L	292	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	F	598	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	J	106	ARG	NE-CZ-NH1	5.43	123.01	120.30
1	K	308	LEU	CA-CB-CG	5.36	127.63	115.30
1	G	365	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	F	355	LEU	CA-CB-CG	5.32	127.54	115.30
1	J	106	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	L	315	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	D	382	LEU	CB-CG-CD2	-5.28	102.02	111.00
1	E	365	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	D	384	ASP	CB-CG-OD1	5.12	122.91	118.30
1	L	598	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	J	365	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	E	625	LEU	CA-CB-CG	5.05	126.92	115.30
1	J	625	LEU	CA-CB-CG	5.05	126.91	115.30
1	H	401	ARG	NE-CZ-NH2	-5.03	117.79	120.30
1	A	355	LEU	CA-CB-CG	5.02	126.85	115.30
1	H	542	ASP	CB-CG-OD1	5.02	122.82	118.30
1	J	593	ASP	N-CA-CB	-5.01	101.58	110.60



There are no chirality outliers.

All (37) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	275	GLY	Peptide
1	A	592	PHE	Peptide
1	B	275	GLY	Peptide
1	B	581	PRO	Peptide
1	B	592	PHE	Peptide
1	B	600	MET	Peptide
1	C	129	GLY	Peptide
1	C	144	GLY	Peptide
1	C	581	PRO	Peptide
1	C	592	PHE	Peptide
1	C	600	MET	Peptide
1	D	129	GLY	Peptide
1	D	144	GLY	Peptide
1	D	275	GLY	Peptide
1	D	592	PHE	Peptide
1	D	600	MET	Peptide
1	E	275	GLY	Peptide
1	E	592	PHE	Peptide
1	F	275	GLY	Peptide
1	F	562	ASP	Peptide
1	F	592	PHE	Peptide
1	F	600	MET	Peptide
1	G	275	GLY	Peptide
1	G	592	PHE	Peptide
1	H	275	GLY	Peptide
1	H	592	PHE	Peptide
1	I	144	GLY	Peptide
1	J	275	GLY	Peptide
1	J	592	PHE	Peptide
1	J	600	MET	Peptide
1	K	144	GLY	Peptide
1	K	275	GLY	Peptide
1	K	562	ASP	Peptide
1	K	581	PRO	Peptide
1	K	592	PHE	Peptide
1	L	275	GLY	Peptide
1	L	592	PHE	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	4560	0	4408	91	0
1	B	4560	0	4408	74	0
1	C	4560	0	4408	63	0
1	D	4560	0	4408	86	0
1	E	4560	0	4408	72	0
1	F	4560	0	4408	75	0
1	G	4560	0	4408	82	0
1	H	4560	0	4408	83	0
1	I	4560	0	4408	94	0
1	J	4560	0	4408	72	0
1	K	4560	0	4408	85	0
1	L	4560	0	4408	92	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
2	D	3	0	0	0	0
2	E	3	0	0	0	0
2	F	3	0	0	0	0
2	G	3	0	0	0	0
2	H	3	0	0	0	0
2	I	3	0	0	0	0
2	J	3	0	0	0	0
2	K	3	0	0	0	0
2	L	3	0	0	0	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	3	0	0	0	0
3	E	3	0	0	0	0
3	F	3	0	0	0	0
3	G	3	0	0	0	0
3	H	3	0	0	0	0
3	I	3	0	0	0	0
3	J	3	0	0	0	0
3	K	3	0	0	0	0
3	L	3	0	0	0	0
4	A	6	0	8	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	6	0	8	0	0
4	C	6	0	8	0	0
4	D	6	0	8	1	0
4	E	6	0	8	0	0
4	F	6	0	8	0	0
4	G	6	0	8	0	0
4	H	6	0	8	1	0
4	I	6	0	8	0	0
4	J	6	0	8	0	0
4	K	6	0	8	2	0
4	L	6	0	8	0	0
5	A	354	0	0	10	0
5	B	362	0	0	10	0
5	C	398	0	0	11	0
5	D	386	0	0	8	0
5	E	357	0	0	9	0
5	F	361	0	0	9	0
5	G	359	0	0	9	0
5	H	376	0	0	12	0
5	I	330	0	0	14	0
5	J	388	0	0	12	0
5	K	359	0	0	9	0
5	L	347	0	0	10	0
All	All	59241	0	52992	898	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 8.

All (898) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:472:GLN:N	1:J:472:GLN:OE1	1.57	1.34
1:L:138:THR:HG22	1:L:401:ARG:NH1	1.42	1.32
1:L:138:THR:CG2	1:L:401:ARG:NH1	2.04	1.20
1:L:555:THR:HG22	5:L:3298:HOH:O	1.49	1.12
1:K:494:THR:HG22	5:K:684:HOH:O	1.52	1.07
1:K:197:GLN:HE21	1:K:219:THR:HG21	1.14	1.06
1:B:473:VAL:HG22	1:B:474:PRO:HD2	1.32	1.06
1:F:138:THR:CG2	1:F:401:ARG:NH1	2.21	1.03
1:F:138:THR:HG22	1:F:401:ARG:NH1	1.74	1.03
1:I:112:ARG:HD3	5:I:1455:HOH:O	1.59	1.01

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:138:THR:CG2	1:I:401:ARG:HH11	1.76	0.99
1:B:473:VAL:HG22	1:B:474:PRO:CD	1.93	0.98
1:G:556:PRO:HD2	5:G:4378:HOH:O	1.64	0.97
1:G:132:GLY:O	1:G:397:LEU:HD21	1.63	0.97
1:F:138:THR:HG22	1:F:401:ARG:HH11	1.26	0.96
1:J:138:THR:HG22	1:J:401:ARG:NH1	1.79	0.96
1:G:413:THR:HG21	1:G:415:GLU:HG3	1.48	0.95
1:J:138:THR:HG22	1:J:401:ARG:HH11	1.30	0.95
1:L:138:THR:HG22	1:L:401:ARG:HH11	1.00	0.95
1:G:112:ARG:HD3	5:G:2482:HOH:O	1.67	0.94
1:D:480:GLN:H	1:D:553:THR:HG21	1.31	0.93
1:A:209:ARG:NH1	1:A:610:ASP:HB3	1.84	0.93
1:I:627:PHE:O	1:I:628:ASP:HB2	1.65	0.92
1:A:209:ARG:NH1	1:A:610:ASP:CB	2.32	0.92
1:I:138:THR:HG22	1:I:401:ARG:HH11	1.35	0.91
1:C:427:GLY:HA2	5:C:4358:HOH:O	1.69	0.91
1:C:627:PHE:O	1:C:628:ASP:HB2	1.69	0.91
1:L:138:THR:CG2	1:L:401:ARG:HH11	1.76	0.89
1:A:209:ARG:HH12	1:A:610:ASP:HB3	1.35	0.89
1:B:112:ARG:HD3	5:B:1043:HOH:O	1.71	0.89
1:G:412:GLU:HG3	5:G:3026:HOH:O	1.71	0.88
1:H:472:GLN:O	1:H:473:VAL:HG23	1.74	0.88
1:C:432:MET:H	1:C:534:GLN:HE22	1.22	0.87
1:I:209:ARG:NH1	1:I:610:ASP:HB3	1.89	0.87
1:G:574:HIS:HD2	5:G:2039:HOH:O	1.55	0.87
1:I:138:THR:CG2	1:I:401:ARG:NH1	2.37	0.87
1:L:473:VAL:HB	1:L:474:PRO:HA	1.57	0.87
1:I:413:THR:HG22	1:I:415:GLU:H	1.41	0.85
1:B:334:HIS:HD2	5:B:2420:HOH:O	1.60	0.85
1:G:209:ARG:NH1	1:G:610:ASP:HB3	1.92	0.85
1:C:144:GLY:HA3	5:C:4092:HOH:O	1.77	0.85
1:G:413:THR:HG22	1:G:414:CYS:H	1.42	0.85
1:K:138:THR:HG22	1:K:401:ARG:HH21	1.40	0.85
1:C:432:MET:H	1:C:534:GLN:NE2	1.75	0.84
1:K:432:MET:H	1:K:534:GLN:NE2	1.76	0.84
1:A:432:MET:H	1:A:534:GLN:NE2	1.76	0.84
1:K:138:THR:CG2	1:K:401:ARG:HH21	1.90	0.83
1:F:138:THR:CG2	1:F:401:ARG:HH11	1.88	0.83
1:E:480:GLN:H	1:E:553:THR:HG21	1.43	0.82
1:K:135:ALA:O	1:K:138:THR:HB	1.79	0.82
1:G:413:THR:CG2	1:G:415:GLU:HG3	2.08	0.82

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:255:ARG:HG3	1:G:255:ARG:HH11	1.42	0.81
1:A:432:MET:H	1:A:534:GLN:HE22	1.25	0.81
1:H:124:VAL:HG11	1:H:142:ARG:HG2	1.64	0.80
1:C:192:ASP:HB2	5:C:1820:HOH:O	1.82	0.79
1:I:508:GLU:HG2	1:I:596:TYR:CE1	2.17	0.79
1:J:138:THR:CG2	1:J:401:ARG:NH1	2.44	0.79
1:A:334:HIS:HD2	5:A:2857:HOH:O	1.64	0.79
1:D:598:ARG:HH22	1:L:499:ASN:HD21	1.29	0.79
1:G:124:VAL:HG11	1:G:142:ARG:HG2	1.65	0.79
1:J:607:GLU:O	1:J:611:MET:HG3	1.82	0.79
1:E:581:PRO:O	1:E:582:GLY:O	2.01	0.79
1:H:466:GLU:HA	5:H:4158:HOH:O	1.83	0.78
1:F:112:ARG:HD3	5:F:2052:HOH:O	1.81	0.78
1:F:135:ALA:O	1:F:138:THR:HB	1.82	0.78
1:J:558:ARG:HB2	5:J:3620:HOH:O	1.82	0.78
1:G:432:MET:H	1:G:534:GLN:NE2	1.82	0.78
1:H:192:ASP:HB2	5:H:3435:HOH:O	1.83	0.77
1:B:538:ARG:HH11	1:B:584:GLN:HE22	1.32	0.77
1:B:472:GLN:O	1:B:473:VAL:HG12	1.84	0.77
1:H:492:ARG:HD3	5:H:3084:HOH:O	1.84	0.76
1:H:431:ARG:HD2	1:H:534:GLN:NE2	2.01	0.76
1:J:472:GLN:N	1:J:472:GLN:CD	2.39	0.75
1:J:192:ASP:HB2	5:J:3674:HOH:O	1.85	0.75
1:D:553:THR:HG23	5:D:1348:HOH:O	1.85	0.75
1:I:255:ARG:HH11	1:I:255:ARG:HG3	1.51	0.75
1:I:375:LEU:HD13	1:I:380:LEU:HD11	1.69	0.75
1:B:574:HIS:HD2	5:B:1279:HOH:O	1.70	0.75
1:D:353:ASP:HA	5:D:2019:HOH:O	1.87	0.75
1:A:147:PRO:O	1:A:149:LYS:HE2	1.86	0.74
1:L:555:THR:CG2	5:L:3298:HOH:O	2.18	0.74
1:B:209:ARG:NH1	1:B:610:ASP:HB3	2.03	0.74
1:K:432:MET:H	1:K:534:GLN:HE22	1.36	0.73
1:A:197:GLN:O	1:A:365:ARG:HD2	1.88	0.73
1:L:432:MET:H	1:L:534:GLN:HE22	1.36	0.73
1:A:473:VAL:HB	1:A:474:PRO:HD3	1.68	0.73
1:L:118:GLU:HG3	5:L:3413:HOH:O	1.88	0.73
1:G:413:THR:HG22	1:G:414:CYS:N	2.03	0.73
1:G:432:MET:H	1:G:534:GLN:HE22	1.37	0.72
1:A:375:LEU:HD13	1:A:380:LEU:HD11	1.70	0.72
1:K:205:MET:O	1:K:206:ASN:HB2	1.90	0.72
1:D:177:ASN:HD21	1:L:598:ARG:H	1.38	0.72

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:63:ARG:HD3	5:H:3738:HOH:O	1.88	0.72
1:F:124:VAL:HG11	1:F:142:ARG:HG2	1.72	0.72
1:I:209:ARG:HD3	1:I:610:ASP:OD2	1.90	0.71
1:E:138:THR:HG22	1:E:401:ARG:HH21	1.54	0.71
1:I:508:GLU:HG2	1:I:596:TYR:HE1	1.56	0.71
1:L:432:MET:H	1:L:534:GLN:NE2	1.88	0.71
1:A:578:PHE:HB3	5:A:3150:HOH:O	1.89	0.71
1:E:236:ASP:HB2	5:E:2752:HOH:O	1.91	0.71
1:L:473:VAL:HG11	1:L:478:VAL:HG11	1.73	0.70
1:C:536:LEU:HD11	1:C:589:MET:HE3	1.73	0.70
1:D:142:ARG:HH21	1:D:147:PRO:HD3	1.56	0.70
1:G:132:GLY:O	1:G:397:LEU:CD2	2.37	0.70
1:D:598:ARG:H	1:L:177:ASN:HD21	1.39	0.70
1:K:591:LYS:HG2	1:K:593:ASP:HB2	1.73	0.70
1:C:536:LEU:HD11	1:C:589:MET:CE	2.21	0.70
1:J:560:ASP:OD1	1:J:562:ASP:HB3	1.91	0.70
1:D:602:HIS:HB3	1:D:614:MET:HG3	1.74	0.70
1:E:135:ALA:O	1:E:138:THR:HB	1.92	0.70
1:H:375:LEU:HD13	1:H:380:LEU:HD11	1.74	0.70
1:E:554:ARG:HG2	1:E:554:ARG:HH11	1.56	0.69
1:J:353:ASP:HA	5:J:1994:HOH:O	1.91	0.69
1:A:177:ASN:HD21	1:I:598:ARG:H	1.41	0.69
1:G:620:MET:SD	1:G:625:LEU:HD12	2.34	0.68
1:F:157:TRP:CE2	1:F:178:ALA:HB3	2.29	0.68
1:A:602:HIS:HB3	1:A:614:MET:HG3	1.75	0.68
1:A:527:HIS:HB2	1:A:577:VAL:HG22	1.76	0.67
1:D:63:ARG:HH12	1:L:63:ARG:NH1	1.92	0.67
1:A:157:TRP:CE2	1:A:178:ALA:HB3	2.28	0.67
1:H:472:GLN:O	1:H:473:VAL:CG2	2.41	0.67
1:K:197:GLN:NE2	1:K:219:THR:HG21	1.99	0.67
1:B:513:GLN:HE21	1:B:536:LEU:HD12	1.60	0.67
1:A:141:GLY:O	1:A:263:LYS:HE3	1.93	0.67
1:H:472:GLN:HA	1:H:472:GLN:NE2	2.07	0.67
1:K:138:THR:CG2	1:K:401:ARG:NH2	2.58	0.67
1:J:451:LYS:HE3	5:J:3397:HOH:O	1.95	0.67
1:F:581:PRO:HG2	1:F:584:GLN:OE1	1.94	0.67
1:A:209:ARG:HH11	1:A:610:ASP:CB	2.06	0.67
1:D:364:GLU:OE2	4:D:5004:GOL:H12	1.95	0.66
1:J:375:LEU:HD13	1:J:380:LEU:HD11	1.77	0.66
1:H:157:TRP:CE2	1:H:178:ALA:HB3	2.30	0.66
1:K:513:GLN:HE21	1:K:536:LEU:HD12	1.60	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:63:ARG:HH22	1:G:63:ARG:NH2	1.94	0.66
1:I:627:PHE:O	1:I:628:ASP:CB	2.43	0.66
1:E:138:THR:CG2	1:E:401:ARG:HH21	2.08	0.66
1:E:607:GLU:O	1:E:611:MET:HG3	1.94	0.66
1:G:627:PHE:O	1:G:628:ASP:HB2	1.96	0.66
1:L:494:THR:HG23	5:L:1773:HOH:O	1.96	0.66
1:C:413:THR:HG22	1:C:414:CYS:H	1.61	0.66
1:G:472:GLN:HA	1:G:472:GLN:OE1	1.94	0.66
1:B:63:ARG:HH11	1:H:63:ARG:NH2	1.94	0.66
1:J:581:PRO:O	1:J:582:GLY:O	2.14	0.65
1:L:461:GLU:O	1:L:494:THR:HG22	1.96	0.65
1:B:115:LYS:HE2	5:B:3104:HOH:O	1.95	0.65
1:F:446:THR:HG21	1:F:460:TRP:CE2	2.31	0.65
1:A:562:ASP:HB3	5:A:1583:HOH:O	1.96	0.65
1:B:607:GLU:O	1:B:611:MET:HG3	1.97	0.65
1:H:63:ARG:CD	5:H:3738:HOH:O	2.44	0.65
1:G:431:ARG:NH1	1:G:534:GLN:HE21	1.95	0.65
1:F:192:ASP:HB2	5:F:4347:HOH:O	1.95	0.65
1:H:209:ARG:NH1	1:H:610:ASP:HB3	2.12	0.65
1:J:157:TRP:CE2	1:J:178:ALA:HB3	2.31	0.65
1:L:112:ARG:HD3	5:L:2483:HOH:O	1.97	0.65
1:L:138:THR:HG21	1:L:401:ARG:NH1	2.10	0.65
1:C:602:HIS:HB3	1:C:614:MET:HG3	1.78	0.65
1:J:255:ARG:HG3	1:J:255:ARG:HH11	1.62	0.65
1:I:521:PRO:HA	1:I:582:GLY:HA3	1.79	0.65
1:I:209:ARG:HH11	1:I:610:ASP:CB	2.09	0.65
1:I:124:VAL:HG11	1:I:142:ARG:HG2	1.79	0.65
1:L:138:THR:HG22	1:L:401:ARG:HH12	1.54	0.65
1:G:209:ARG:HH11	1:G:610:ASP:HB3	1.62	0.64
1:D:333:VAL:HG22	1:D:370:VAL:HG12	1.77	0.64
1:E:70:ARG:NH2	5:E:2468:HOH:O	2.31	0.64
1:E:480:GLN:N	1:E:553:THR:HG21	2.12	0.64
1:G:209:ARG:HH11	1:G:610:ASP:CB	2.09	0.64
1:I:432:MET:H	1:I:534:GLN:NE2	1.96	0.64
1:A:101:ARG:HG3	1:A:193:HIS:O	1.98	0.64
1:I:138:THR:HG22	1:I:401:ARG:NH1	2.05	0.64
1:G:607:GLU:O	1:G:611:MET:HG3	1.98	0.64
1:I:135:ALA:O	1:I:138:THR:HB	1.98	0.64
1:B:209:ARG:HD3	1:B:610:ASP:OD2	1.98	0.64
1:I:209:ARG:HH11	1:I:610:ASP:HB3	1.60	0.64
1:A:473:VAL:HB	1:A:474:PRO:CD	2.27	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:209:ARG:NH1	1:G:610:ASP:CB	2.61	0.63
1:K:197:GLN:HE21	1:K:219:THR:CG2	2.03	0.63
1:D:581:PRO:O	1:D:584:GLN:HB3	1.99	0.63
1:K:219:THR:HG22	1:K:220:TYR:H	1.62	0.63
1:K:553:THR:HG23	1:K:555:THR:O	1.99	0.63
1:L:627:PHE:O	1:L:628:ASP:HB2	1.99	0.63
1:H:322:ILE:HD12	1:H:326:ASP:HA	1.79	0.63
1:I:209:ARG:NH1	1:I:610:ASP:CB	2.62	0.63
1:H:336:ILE:HB	1:H:425:LEU:HD21	1.80	0.62
1:B:627:PHE:O	1:B:628:ASP:HB2	1.99	0.62
1:H:431:ARG:HA	1:H:534:GLN:HE22	1.64	0.62
1:I:456:HIS:CE1	1:I:611:MET:CE	2.82	0.62
1:E:538:ARG:HH11	1:E:584:GLN:HE22	1.47	0.62
1:J:431:ARG:NH1	1:J:572:LEU:O	2.33	0.62
1:F:55:ARG:CZ	5:F:3646:HOH:O	2.47	0.61
1:F:375:LEU:HD13	1:F:380:LEU:HD11	1.80	0.61
1:H:271:ASN:O	1:H:274:THR:O	2.18	0.61
1:H:472:GLN:O	1:H:473:VAL:CB	2.47	0.61
1:J:582:GLY:O	1:J:584:GLN:N	2.32	0.61
1:F:413:THR:HG22	1:F:415:GLU:H	1.66	0.61
1:A:243:ILE:HD13	1:A:308:LEU:HD11	1.83	0.61
1:E:177:ASN:HD21	1:K:598:ARG:H	1.46	0.61
1:K:620:MET:SD	1:K:625:LEU:HD12	2.40	0.61
1:I:255:ARG:HG3	1:I:255:ARG:NH1	2.14	0.61
1:J:138:THR:CG2	1:J:401:ARG:HH11	2.07	0.61
1:D:271:ASN:HD22	1:D:274:THR:H	1.49	0.61
1:E:537:GLY:HA2	1:E:567:LEU:HD21	1.83	0.61
1:J:197:GLN:O	1:J:365:ARG:HD2	2.00	0.61
1:H:413:THR:HG22	1:H:414:CYS:H	1.66	0.61
1:L:375:LEU:HD13	1:L:380:LEU:HD11	1.81	0.61
1:B:325:ASP:O	1:B:326:ASP:HB2	2.01	0.61
1:A:413:THR:HG22	1:A:414:CYS:H	1.63	0.60
1:D:591:LYS:HG2	1:D:593:ASP:HB2	1.83	0.60
1:H:431:ARG:HD2	1:H:534:GLN:HE22	1.66	0.60
1:B:177:ASN:HD21	1:H:598:ARG:H	1.50	0.60
1:I:336:ILE:HB	1:I:425:LEU:HD21	1.83	0.60
1:G:255:ARG:HG3	1:G:255:ARG:NH1	2.15	0.60
1:L:138:THR:CG2	1:L:401:ARG:HH12	2.09	0.60
1:D:271:ASN:HD21	1:D:273:GLU:HB2	1.66	0.60
1:L:157:TRP:CE2	1:L:178:ALA:HB3	2.37	0.60
1:L:346:PRO:HB2	5:L:2770:HOH:O	2.02	0.60

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:138:THR:HG22	1:E:401:ARG:HE	1.65	0.60
1:C:413:THR:HG22	1:C:414:CYS:N	2.17	0.60
1:I:134:PRO:HB3	1:I:138:THR:HG21	1.82	0.60
1:E:520:SER:O	1:E:582:GLY:HA2	2.01	0.59
1:C:334:HIS:HE1	5:C:1397:HOH:O	1.85	0.59
1:I:271:ASN:O	1:I:274:THR:O	2.19	0.59
1:C:139:GLU:HG2	5:C:3035:HOH:O	2.02	0.59
1:D:558:ARG:HD2	5:D:3558:HOH:O	2.01	0.59
1:G:375:LEU:HD13	1:G:380:LEU:HD11	1.83	0.59
1:F:142:ARG:HH21	1:F:147:PRO:HD3	1.67	0.59
1:K:364:GLU:OE2	4:K:5011:GOL:H12	2.02	0.59
1:L:536:LEU:HD11	1:L:589:MET:CE	2.32	0.59
1:C:157:TRP:CE2	1:C:178:ALA:HB3	2.37	0.59
1:I:581:PRO:O	1:I:582:GLY:O	2.21	0.59
1:K:571:GLU:O	1:K:571:GLU:HG2	2.03	0.59
1:G:397:LEU:HB2	5:G:1378:HOH:O	2.02	0.59
1:H:520:SER:HB2	1:H:521:PRO:HD2	1.84	0.59
1:B:322:ILE:HD12	1:B:326:ASP:HA	1.83	0.59
1:F:379:ARG:HG2	1:F:409:ARG:HG2	1.84	0.59
1:F:413:THR:HG22	1:F:414:CYS:N	2.18	0.59
1:D:346:PRO:HG3	1:D:425:LEU:HG	1.85	0.59
1:E:205:MET:CE	1:E:498:PHE:CE1	2.86	0.59
1:K:602:HIS:HB3	1:K:614:MET:HG3	1.85	0.58
1:B:209:ARG:HH11	1:B:610:ASP:CB	2.17	0.58
1:D:538:ARG:HH11	1:D:584:GLN:HE22	1.51	0.58
1:G:431:ARG:NH1	1:G:534:GLN:NE2	2.51	0.58
1:B:465:VAL:HG12	1:B:490:THR:HG22	1.86	0.58
1:D:63:ARG:HH12	1:L:63:ARG:HH11	1.50	0.58
1:J:473:VAL:HG12	1:J:478:VAL:HG11	1.83	0.58
1:L:334:HIS:HD2	5:L:3995:HOH:O	1.85	0.58
1:C:177:ASN:HD21	1:G:598:ARG:H	1.51	0.58
1:E:245:ASP:O	1:E:246:ARG:HD3	2.04	0.58
1:A:577:VAL:HG12	1:A:577:VAL:O	2.02	0.58
1:C:197:GLN:O	1:C:365:ARG:HD2	2.02	0.58
1:A:334:HIS:HE1	5:A:1927:HOH:O	1.85	0.58
1:D:142:ARG:HE	1:D:147:PRO:HD3	1.67	0.58
1:D:432:MET:H	1:D:534:GLN:NE2	2.02	0.58
1:D:443:ILE:HD11	1:D:504:PHE:CE2	2.39	0.58
1:D:480:GLN:N	1:D:553:THR:HG21	2.12	0.58
1:D:443:ILE:HD11	1:D:504:PHE:CZ	2.38	0.58
1:E:432:MET:H	1:E:534:GLN:NE2	2.01	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:536:LEU:HD11	1:F:589:MET:HE3	1.85	0.58
1:L:271:ASN:HD22	1:L:274:THR:H	1.52	0.58
1:H:607:GLU:O	1:H:611:MET:HG3	2.04	0.58
1:K:582:GLY:N	5:K:661:HOH:O	2.24	0.58
1:A:365:ARG:NH2	1:A:576:ASP:OD1	2.35	0.57
1:C:276:LYS:HB2	1:C:277:PRO:HD2	1.85	0.57
1:C:582:GLY:N	5:C:869:HOH:O	2.37	0.57
1:E:138:THR:CG2	1:E:401:ARG:NH2	2.67	0.57
1:H:451:LYS:HE2	1:H:476:GLU:OE1	2.04	0.57
1:B:177:ASN:HD22	1:H:597:GLY:HA3	1.68	0.57
1:C:352:ASP:CG	1:C:353:ASP:H	2.06	0.57
1:K:413:THR:HG22	1:K:415:GLU:H	1.68	0.57
1:B:473:VAL:CG2	1:B:474:PRO:HD2	2.22	0.57
1:H:523:LEU:C	1:H:523:LEU:HD23	2.23	0.57
1:H:627:PHE:O	1:H:628:ASP:HB3	2.04	0.57
1:A:523:LEU:HD21	1:A:579:GLN:HB3	1.86	0.57
1:J:112:ARG:HD3	5:J:2162:HOH:O	2.05	0.57
1:F:581:PRO:O	1:F:582:GLY:O	2.23	0.57
1:F:602:HIS:HB3	1:F:614:MET:HG3	1.87	0.57
1:J:135:ALA:O	1:J:138:THR:HB	2.04	0.57
1:E:472:GLN:N	1:E:472:GLN:OE1	2.38	0.57
1:L:536:LEU:HD11	1:L:589:MET:HE3	1.86	0.57
1:A:598:ARG:H	1:I:177:ASN:HD21	1.51	0.57
1:D:255:ARG:HH11	1:E:345:ARG:NH1	2.01	0.57
1:G:157:TRP:CE2	1:G:178:ALA:HB3	2.40	0.57
1:K:413:THR:HG22	1:K:414:CYS:N	2.20	0.57
1:A:327:ARG:HD2	5:A:2261:HOH:O	2.04	0.57
1:C:598:ARG:H	1:G:177:ASN:HD21	1.53	0.57
1:E:194:GLN:NE2	5:E:1962:HOH:O	2.37	0.57
1:E:205:MET:HE3	1:E:498:PHE:CE1	2.40	0.57
1:E:205:MET:O	1:E:206:ASN:HB2	2.02	0.57
1:F:197:GLN:O	1:F:365:ARG:HD2	2.03	0.57
1:H:431:ARG:HH11	1:H:534:GLN:HE21	1.51	0.57
1:F:68:ALA:HB1	1:F:112:ARG:HG3	1.87	0.57
1:G:197:GLN:O	1:G:365:ARG:HD2	2.05	0.56
5:I:669:HOH:O	1:J:423:GLU:HG3	2.05	0.56
1:G:209:ARG:HD3	1:G:610:ASP:OD2	2.05	0.56
1:H:402:TYR:HB3	1:H:404:GLU:OE2	2.05	0.56
1:D:177:ASN:ND2	1:L:597:GLY:HA3	2.21	0.56
1:I:334:HIS:HE1	5:I:692:HOH:O	1.87	0.56
1:J:537:GLY:HA2	1:J:567:LEU:HD21	1.87	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:159:VAL:HB	1:K:178:ALA:HA	1.88	0.56
1:L:271:ASN:O	1:L:274:THR:O	2.23	0.56
1:E:197:GLN:O	1:E:365:ARG:HD2	2.05	0.56
1:I:143:GLY:HA3	5:I:3277:HOH:O	2.05	0.56
1:K:209:ARG:NH1	1:K:610:ASP:HB3	2.18	0.56
1:B:115:LYS:CE	5:B:3104:HOH:O	2.53	0.56
1:B:177:ASN:ND2	1:H:597:GLY:HA3	2.21	0.56
1:E:325:ASP:O	1:E:326:ASP:HB2	2.05	0.56
1:E:485:ASP:OD1	1:E:485:ASP:C	2.44	0.56
1:I:197:GLN:O	1:I:365:ARG:HD2	2.05	0.56
1:C:432:MET:N	1:C:534:GLN:HE22	1.98	0.55
1:K:611:MET:HG2	5:K:2639:HOH:O	2.06	0.55
1:B:473:VAL:HG22	1:B:474:PRO:HD3	1.84	0.55
1:E:112:ARG:HD3	5:E:1825:HOH:O	2.05	0.55
1:H:276:LYS:HG3	1:H:277:PRO:HD2	1.88	0.55
1:C:336:ILE:HB	1:C:425:LEU:HD21	1.88	0.55
1:L:197:GLN:O	1:L:365:ARG:HD2	2.06	0.55
1:E:138:THR:CG2	1:E:401:ARG:HE	2.20	0.55
1:C:63:ARG:HH22	1:G:63:ARG:HH21	1.54	0.55
1:E:255:ARG:HH11	1:E:255:ARG:HG2	1.71	0.55
1:G:555:THR:O	5:G:787:HOH:O	2.18	0.55
1:L:135:ALA:O	1:L:138:THR:HB	2.07	0.55
1:I:159:VAL:HB	1:I:178:ALA:HA	1.88	0.55
1:K:157:TRP:CE2	1:K:178:ALA:HB3	2.42	0.55
1:K:197:GLN:O	1:K:365:ARG:HD2	2.07	0.55
1:L:523:LEU:C	1:L:523:LEU:HD23	2.27	0.55
1:E:80:LEU:HB3	1:E:81:PRO:HD2	1.89	0.55
1:H:197:GLN:O	1:H:365:ARG:HD2	2.07	0.55
1:A:85:MET:HB3	1:A:214:ALA:O	2.07	0.55
1:B:413:THR:HG22	1:B:414:CYS:N	2.22	0.55
1:E:112:ARG:CD	5:E:1825:HOH:O	2.55	0.55
1:A:142:ARG:HD3	1:A:249:ASP:OD2	2.07	0.54
1:D:336:ILE:HB	1:D:425:LEU:HD11	1.90	0.54
1:A:333:VAL:HG22	1:A:370:VAL:HG12	1.89	0.54
1:F:159:VAL:HB	1:F:178:ALA:HA	1.89	0.54
1:D:627:PHE:O	1:D:628:ASP:HB2	2.07	0.54
1:E:138:THR:HG22	1:E:401:ARG:NH2	2.21	0.54
1:L:336:ILE:HB	1:L:425:LEU:HD21	1.89	0.54
1:L:473:VAL:HB	1:L:474:PRO:CA	2.32	0.54
1:A:115:LYS:HE2	5:A:3659:HOH:O	2.07	0.54
1:B:472:GLN:N	1:B:472:GLN:CD	2.60	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:255:ARG:HG3	1:C:255:ARG:HH11	1.72	0.54
1:C:352:ASP:OD1	1:C:353:ASP:N	2.38	0.54
1:A:209:ARG:NH1	1:A:610:ASP:HB2	2.22	0.54
1:E:176:ASP:OD2	1:K:598:ARG:HD2	2.08	0.54
1:E:554:ARG:HG2	1:E:554:ARG:NH1	2.23	0.54
1:K:163:HIS:CE1	1:K:527:HIS:CE1	2.95	0.54
1:A:598:ARG:HH12	1:I:499:ASN:HD21	1.56	0.54
1:D:124:VAL:HG11	1:D:142:ARG:HG2	1.89	0.54
1:D:142:ARG:HH21	1:D:147:PRO:CD	2.21	0.54
1:F:598:ARG:H	1:J:177:ASN:HD21	1.56	0.54
1:I:520:SER:O	1:I:582:GLY:HA2	2.08	0.54
1:B:413:THR:HG22	1:B:414:CYS:H	1.70	0.54
1:F:536:LEU:HD11	1:F:589:MET:CE	2.38	0.54
1:H:413:THR:HG22	1:H:414:CYS:N	2.22	0.54
1:H:432:MET:H	1:H:534:GLN:NE2	2.06	0.54
1:E:433:SER:O	1:E:436:ILE:HG22	2.09	0.53
1:H:602:HIS:HB3	1:H:614:MET:HG3	1.89	0.53
1:K:142:ARG:HD3	1:K:249:ASP:OD2	2.07	0.53
1:A:146:GLU:HG2	5:A:1161:HOH:O	2.07	0.53
1:C:176:ASP:OD1	1:G:598:ARG:HD2	2.07	0.53
1:F:627:PHE:O	1:F:628:ASP:HB3	2.08	0.53
1:I:456:HIS:CE1	1:I:611:MET:HE1	2.43	0.53
1:A:271:ASN:HD22	1:A:274:THR:H	1.55	0.53
1:F:521:PRO:HA	1:F:583:PRO:HD3	1.89	0.53
1:B:334:HIS:HE1	5:B:689:HOH:O	1.90	0.53
1:G:205:MET:HE1	1:G:498:PHE:CE1	2.43	0.53
1:I:157:TRP:CE2	1:I:178:ALA:HB3	2.43	0.53
1:C:325:ASP:O	1:C:326:ASP:HB2	2.09	0.53
1:J:193:HIS:NE2	1:J:532:ASP:OD2	2.28	0.53
1:A:365:ARG:HH22	1:A:576:ASP:CG	2.12	0.53
1:H:237:ARG:HD3	5:H:970:HOH:O	2.09	0.53
1:H:523:LEU:HD23	1:H:524:HIS:N	2.24	0.53
1:A:547:ASP:HB3	1:A:550:LEU:HB3	1.90	0.53
1:D:322:ILE:HD12	1:D:326:ASP:HA	1.90	0.53
1:E:473:VAL:HG23	1:E:474:PRO:HA	1.91	0.53
1:B:63:ARG:HD3	1:H:63:ARG:NH2	2.24	0.53
1:A:255:ARG:HG3	1:A:255:ARG:HH11	1.73	0.53
1:L:404:GLU:CD	1:L:404:GLU:H	2.12	0.53
1:B:176:ASP:O	1:H:597:GLY:HA2	2.09	0.52
1:H:163:HIS:C	1:H:163:HIS:CD2	2.81	0.52
1:F:63:ARG:NH2	1:J:63:ARG:HD3	2.25	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:432:MET:H	1:E:534:GLN:HE22	1.57	0.52
1:B:584:GLN:HB2	5:B:1416:HOH:O	2.09	0.52
1:H:356:PRO:HD2	5:H:2523:HOH:O	2.09	0.52
1:A:472:GLN:CD	1:A:472:GLN:O	2.48	0.52
1:D:352:ASP:OD2	1:D:353:ASP:N	2.42	0.52
1:F:521:PRO:HA	1:F:582:GLY:HA3	1.90	0.52
1:A:498:PHE:HA	1:A:614:MET:O	2.09	0.52
1:A:513:GLN:HE21	1:A:536:LEU:HD12	1.73	0.52
1:F:138:THR:HG21	1:F:401:ARG:NH1	2.21	0.52
1:D:177:ASN:HD22	1:L:597:GLY:CA	2.23	0.52
1:F:325:ASP:O	1:F:326:ASP:HB2	2.08	0.52
1:I:602:HIS:HB3	1:I:614:MET:HG3	1.91	0.52
1:C:124:VAL:HG11	1:C:142:ARG:HG2	1.90	0.52
1:K:336:ILE:HB	1:K:425:LEU:HD11	1.92	0.52
1:E:54:LEU:HD11	5:E:3984:HOH:O	2.10	0.52
1:L:472:GLN:HG3	1:L:473:VAL:HG13	1.92	0.52
1:K:112:ARG:HD3	5:K:1644:HOH:O	2.09	0.51
1:D:177:ASN:HD22	1:L:597:GLY:HA3	1.74	0.51
1:F:355:LEU:HD22	1:F:569:PRO:HG2	1.91	0.51
1:G:255:ARG:HH11	1:G:255:ARG:CG	2.15	0.51
1:G:336:ILE:HB	1:G:425:LEU:HD21	1.93	0.51
1:I:301:ASP:OD1	1:I:413:THR:HB	2.10	0.51
1:I:591:LYS:HE2	1:I:593:ASP:OD1	2.11	0.51
1:J:255:ARG:HG3	1:J:255:ARG:NH1	2.25	0.51
1:D:325:ASP:O	1:D:326:ASP:HB2	2.10	0.51
1:F:91:GLN:NE2	5:F:3521:HOH:O	2.42	0.51
1:A:591:LYS:HE3	5:A:4191:HOH:O	2.10	0.51
1:B:209:ARG:NH1	1:B:610:ASP:CB	2.71	0.51
1:G:68:ALA:HB1	1:G:112:ARG:HG3	1.93	0.51
1:E:431:ARG:NH2	1:E:572:LEU:O	2.42	0.51
1:J:482:THR:HG1	1:J:488:THR:HG1	1.50	0.51
1:I:533:PHE:HB3	1:I:588:VAL:HG22	1.92	0.51
1:K:494:THR:CG2	5:K:684:HOH:O	2.30	0.51
1:L:68:ALA:HB1	1:L:112:ARG:HG3	1.93	0.51
1:C:581:PRO:O	1:C:582:GLY:O	2.28	0.51
1:D:531:ALA:HB3	1:D:533:PHE:CE1	2.46	0.51
1:D:581:PRO:HG2	1:D:584:GLN:OE1	2.10	0.51
1:H:209:ARG:NH1	1:H:610:ASP:CB	2.74	0.51
1:K:591:LYS:HE2	1:K:593:ASP:OD1	2.10	0.51
1:K:598:ARG:NH2	5:K:2199:HOH:O	2.44	0.51
1:A:536:LEU:HD11	1:A:589:MET:HE3	1.92	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:531:ALA:HB3	1:B:533:PHE:CE1	2.46	0.51
1:G:472:GLN:OE1	1:G:472:GLN:CA	2.59	0.51
1:J:536:LEU:HD11	1:J:589:MET:HE3	1.91	0.51
1:K:237:ARG:HD3	5:K:2479:HOH:O	2.11	0.51
1:A:163:HIS:CE1	1:A:363:ALA:HB1	2.45	0.50
1:B:598:ARG:H	1:H:177:ASN:HD21	1.57	0.50
1:G:538:ARG:HH11	1:G:584:GLN:HE22	1.58	0.50
1:B:584:GLN:HG2	1:B:585:GLY:N	2.25	0.50
1:C:176:ASP:O	1:G:597:GLY:HA2	2.11	0.50
1:D:274:THR:HB	1:D:276:LYS:HD2	1.94	0.50
1:I:432:MET:H	1:I:534:GLN:HE22	1.56	0.50
1:K:531:ALA:HB3	1:K:533:PHE:CE1	2.46	0.50
1:A:186:LEU:HD11	1:I:106:ARG:HG2	1.94	0.50
1:A:209:ARG:HH11	1:A:610:ASP:CG	2.15	0.50
1:B:536:LEU:HD11	1:B:589:MET:HE3	1.92	0.50
1:D:271:ASN:O	1:D:274:THR:O	2.30	0.50
1:I:346:PRO:HD3	1:I:425:LEU:HB2	1.93	0.50
1:A:337:GLY:N	1:A:367:ASP:HB3	2.27	0.50
1:B:375:LEU:HD13	1:B:380:LEU:HD11	1.93	0.50
1:E:205:MET:HE3	1:E:498:PHE:HE1	1.76	0.50
1:H:325:ASP:O	1:H:326:ASP:HB2	2.12	0.50
1:J:269:GLN:O	5:J:3871:HOH:O	2.18	0.50
1:J:346:PRO:HD3	1:J:425:LEU:HB2	1.94	0.50
1:B:205:MET:O	1:B:206:ASN:HB2	2.12	0.50
1:B:446:THR:HG21	1:B:460:TRP:CE2	2.47	0.50
1:C:159:VAL:HB	1:C:178:ALA:HA	1.94	0.50
1:I:138:THR:HG21	1:I:401:ARG:NH1	2.24	0.50
1:J:205:MET:O	1:J:206:ASN:HB2	2.11	0.50
1:A:271:ASN:O	1:A:274:THR:O	2.29	0.50
1:C:499:ASN:ND2	1:G:598:ARG:HH22	2.09	0.50
1:H:125:GLU:HG2	1:H:264:THR:OG1	2.12	0.50
1:I:451:LYS:NZ	1:I:476:GLU:OE1	2.35	0.50
1:F:177:ASN:HD22	1:J:597:GLY:HA3	1.77	0.50
1:D:627:PHE:O	1:D:628:ASP:CB	2.60	0.50
1:H:587:ARG:NH1	5:H:1191:HOH:O	2.37	0.50
1:F:177:ASN:HD21	1:J:598:ARG:H	1.60	0.50
1:G:255:ARG:NH1	1:G:255:ARG:CG	2.73	0.50
1:K:464:GLU:OE2	1:K:489:LYS:HD3	2.12	0.50
1:L:245:ASP:OD2	1:L:315:ARG:HD2	2.12	0.50
1:L:545:GLY:HA3	1:L:555:THR:O	2.11	0.50
1:F:70:ARG:NH2	5:F:2951:HOH:O	2.44	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:199:TRP:HA	1:H:219:THR:HA	1.94	0.49
1:J:124:VAL:HG11	1:J:142:ARG:HG2	1.94	0.49
1:K:537:GLY:HA2	1:K:567:LEU:HD21	1.93	0.49
1:B:472:GLN:O	1:B:473:VAL:O	2.30	0.49
1:B:554:ARG:HG2	1:B:554:ARG:HH11	1.77	0.49
1:D:197:GLN:O	1:D:365:ARG:HD2	2.12	0.49
1:F:443:ILE:HD12	1:F:443:ILE:N	2.27	0.49
1:G:598:ARG:NH2	5:G:1346:HOH:O	2.45	0.49
1:D:70:ARG:HD2	5:D:2882:HOH:O	2.12	0.49
1:D:271:ASN:ND2	1:D:273:GLU:HB2	2.27	0.49
1:F:432:MET:H	1:F:534:GLN:NE2	2.10	0.49
1:F:538:ARG:HH11	1:F:584:GLN:HE22	1.59	0.49
1:I:126:VAL:HG13	1:I:127:PRO:HD2	1.94	0.49
1:B:473:VAL:CG2	1:B:474:PRO:CD	2.78	0.49
1:G:620:MET:SD	1:G:625:LEU:CD1	3.01	0.49
1:I:431:ARG:NH1	1:I:572:LEU:O	2.45	0.49
1:D:584:GLN:HG2	1:D:585:GLY:N	2.28	0.49
1:L:362:PRO:O	1:L:363:ALA:HB3	2.13	0.49
1:E:598:ARG:H	1:K:177:ASN:HD21	1.58	0.49
1:F:520:SER:O	1:F:582:GLY:HA2	2.10	0.49
1:K:316:ILE:HD11	1:K:523:LEU:HD22	1.94	0.49
1:D:538:ARG:HH11	1:D:584:GLN:NE2	2.11	0.49
1:G:86:TRP:CD2	1:G:113:ILE:HD13	2.48	0.49
1:I:83:THR:HG23	1:I:258:GLY:O	2.12	0.49
1:I:500:ASP:HB3	5:I:1771:HOH:O	2.11	0.49
1:K:431:ARG:NH2	1:K:535:VAL:O	2.45	0.49
1:L:128:LEU:HD23	1:L:265:VAL:HG11	1.93	0.49
1:A:197:GLN:O	1:A:365:ARG:CD	2.61	0.49
1:G:337:GLY:N	1:G:367:ASP:HB3	2.27	0.49
1:K:431:ARG:HD2	1:K:534:GLN:NE2	2.28	0.49
1:D:597:GLY:HA3	1:L:177:ASN:ND2	2.28	0.49
1:F:150:ASP:OD2	1:J:626:LYS:HD2	2.13	0.49
1:I:485:ASP:C	1:I:485:ASP:OD1	2.51	0.49
1:J:70:ARG:HD2	5:J:1838:HOH:O	2.13	0.49
1:D:161:HIS:NE2	1:D:163:HIS:HA	2.28	0.48
1:G:397:LEU:HD23	1:G:397:LEU:HA	1.67	0.48
1:L:86:TRP:CD2	1:L:113:ILE:HD13	2.48	0.48
1:D:597:GLY:HA3	1:L:177:ASN:HD22	1.77	0.48
1:J:142:ARG:HH21	1:J:147:PRO:HD3	1.77	0.48
1:L:434:HIS:CD2	1:L:438:HIS:CE1	3.01	0.48
1:F:150:ASP:CG	1:J:626:LYS:HD2	2.34	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:VAL:HB	1:A:178:ALA:HA	1.95	0.48
1:B:194:GLN:NE2	5:B:4570:HOH:O	2.41	0.48
1:B:209:ARG:HH11	1:B:610:ASP:HB3	1.70	0.48
1:C:149:LYS:HG2	5:C:1112:HOH:O	2.13	0.48
1:C:443:ILE:HD11	1:C:504:PHE:CE2	2.48	0.48
1:G:175:ALA:HB3	1:G:205:MET:HE2	1.95	0.48
1:A:336:ILE:HB	1:A:425:LEU:HD11	1.96	0.48
1:G:555:THR:HB	1:G:556:PRO:CD	2.43	0.48
1:B:532:ASP:HB3	5:B:1279:HOH:O	2.13	0.48
1:D:584:GLN:HB2	5:D:4134:HOH:O	2.14	0.48
1:H:446:THR:HG21	1:H:460:TRP:CE2	2.49	0.48
1:J:159:VAL:HB	1:J:178:ALA:HA	1.94	0.48
1:K:219:THR:OG1	1:K:242:LEU:HD21	2.14	0.48
1:E:205:MET:HE1	1:E:498:PHE:CE1	2.48	0.48
1:F:243:ILE:HG22	1:F:289:VAL:HG22	1.96	0.48
1:G:124:VAL:CG1	1:G:142:ARG:HG2	2.41	0.48
1:H:209:ARG:HH11	1:H:610:ASP:CB	2.26	0.48
1:F:598:ARG:HD2	1:J:176:ASP:OD1	2.13	0.48
1:G:355:LEU:HD11	5:G:1116:HOH:O	2.14	0.48
1:H:482:THR:HA	1:H:487:ARG:O	2.13	0.48
1:J:520:SER:HB2	1:J:521:PRO:HD2	1.95	0.48
1:A:499:ASN:HD21	1:I:598:ARG:HH12	1.61	0.48
1:C:627:PHE:O	1:C:628:ASP:CB	2.53	0.48
1:E:63:ARG:NH1	1:K:60:GLU:OE1	2.47	0.48
1:E:177:ASN:HD22	1:K:597:GLY:HA3	1.77	0.48
1:E:601:TYR:CE2	1:E:615:ARG:HB2	2.49	0.48
1:F:461:GLU:HG2	1:F:504:PHE:CZ	2.48	0.48
1:I:236:ASP:HB2	5:I:1012:HOH:O	2.14	0.48
1:J:465:VAL:HG12	1:J:466:GLU:N	2.28	0.48
1:L:69:LEU:N	1:L:69:LEU:HD12	2.29	0.48
1:G:334:HIS:HE1	5:G:1009:HOH:O	1.97	0.47
1:I:542:ASP:HA	5:I:4225:HOH:O	2.14	0.47
1:K:523:LEU:HD23	1:K:523:LEU:C	2.34	0.47
1:A:627:PHE:O	1:A:628:ASP:HB3	2.14	0.47
1:H:194:GLN:NE2	5:H:2938:HOH:O	2.34	0.47
1:J:37:ALA:HB3	1:J:40:GLU:OE1	2.14	0.47
1:J:578:PHE:HB3	5:J:1556:HOH:O	2.13	0.47
1:A:177:ASN:ND2	1:I:598:ARG:H	2.11	0.47
1:B:431:ARG:HA	1:B:534:GLN:HE22	1.79	0.47
1:D:498:PHE:HA	1:D:614:MET:O	2.14	0.47
1:E:443:ILE:HD11	1:E:504:PHE:CZ	2.48	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:533:PHE:HB2	1:I:578:PHE:HZ	1.79	0.47
1:D:280:ILE:HB	1:D:281:PRO:CD	2.44	0.47
1:E:554:ARG:NH1	1:E:554:ARG:CG	2.76	0.47
1:A:413:THR:HG22	1:A:414:CYS:N	2.27	0.47
1:B:459:ILE:HG13	1:B:613:MET:HG3	1.96	0.47
1:B:492:ARG:HG3	1:B:492:ARG:HH11	1.80	0.47
1:E:68:ALA:HB1	1:E:112:ARG:HG3	1.97	0.47
1:H:159:VAL:HB	1:H:178:ALA:HA	1.95	0.47
1:H:558:ARG:NH1	5:H:1505:HOH:O	2.45	0.47
1:J:148:ASN:OD1	1:J:150:ASP:HB2	2.13	0.47
1:L:472:GLN:C	1:L:473:VAL:HG13	2.34	0.47
1:A:442:LEU:C	1:A:443:ILE:HD13	2.35	0.47
1:C:498:PHE:HA	1:C:614:MET:O	2.15	0.47
1:D:142:ARG:NH2	1:D:147:PRO:HD3	2.27	0.47
1:K:413:THR:HG22	1:K:415:GLU:N	2.29	0.47
1:D:499:ASN:ND2	1:L:598:ARG:HH22	2.12	0.47
1:D:597:GLY:CA	1:L:177:ASN:HD22	2.28	0.47
1:E:553:THR:HG23	5:E:1305:HOH:O	2.13	0.47
1:F:64:GLU:OE2	1:J:64:GLU:OE2	2.32	0.47
1:H:498:PHE:HA	1:H:614:MET:O	2.15	0.47
1:H:568:ALA:HB3	1:H:571:GLU:HG2	1.96	0.47
1:J:115:LYS:NZ	5:J:3059:HOH:O	2.35	0.47
1:K:431:ARG:HD2	1:K:534:GLN:HE22	1.79	0.47
1:L:318:ASN:HB3	1:L:357:VAL:HG11	1.97	0.47
1:L:325:ASP:O	1:L:326:ASP:HB2	2.14	0.47
1:A:545:GLY:HA3	1:A:555:THR:O	2.13	0.47
1:C:598:ARG:HD2	1:G:176:ASP:OD2	2.15	0.47
1:E:159:VAL:HB	1:E:178:ALA:HA	1.96	0.47
1:I:325:ASP:O	1:I:326:ASP:HB2	2.15	0.47
1:J:498:PHE:HA	1:J:614:MET:O	2.15	0.47
1:D:280:ILE:HB	1:D:281:PRO:HD2	1.97	0.47
1:C:63:ARG:NH2	1:G:63:ARG:NH2	2.63	0.47
1:D:68:ALA:HB1	1:D:112:ARG:HG3	1.97	0.47
1:D:159:VAL:HB	1:D:178:ALA:HA	1.97	0.47
1:E:243:ILE:HD13	1:E:308:LEU:HD11	1.97	0.47
1:G:555:THR:HB	1:G:556:PRO:HD3	1.97	0.47
1:H:124:VAL:CG1	1:H:142:ARG:HG2	2.41	0.47
1:I:134:PRO:HG3	1:I:396:PRO:HB2	1.97	0.47
1:C:492:ARG:NH1	5:C:2755:HOH:O	2.48	0.46
1:K:485:ASP:OD1	1:K:487:ARG:HB3	2.14	0.46
1:K:538:ARG:HH11	1:K:584:GLN:HE22	1.62	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:138:THR:CG2	1:E:401:ARG:NE	2.78	0.46
1:F:163:HIS:CE1	1:F:363:ALA:HB1	2.51	0.46
1:F:523:LEU:HD23	1:F:523:LEU:C	2.36	0.46
1:G:250:THR:HA	1:G:255:ARG:O	2.16	0.46
1:G:620:MET:HE2	1:G:624:ALA:HB3	1.97	0.46
1:H:538:ARG:HH11	1:H:584:GLN:HE22	1.62	0.46
1:H:591:LYS:HG2	1:H:593:ASP:HB2	1.97	0.46
1:I:255:ARG:NH1	1:I:255:ARG:CG	2.78	0.46
1:K:197:GLN:O	1:K:365:ARG:CD	2.64	0.46
1:D:487:ARG:HB2	1:D:487:ARG:CZ	2.45	0.46
1:F:413:THR:HG22	1:F:414:CYS:H	1.79	0.46
1:G:562:ASP:O	1:G:564:PRO:HD3	2.15	0.46
1:K:482:THR:HA	1:K:487:ARG:O	2.15	0.46
1:L:285:PRO:HG2	1:L:286:TYR:CE1	2.50	0.46
1:D:499:ASN:HD21	1:L:598:ARG:HH22	1.62	0.46
1:E:538:ARG:HH11	1:E:584:GLN:NE2	2.12	0.46
1:F:473:VAL:HG11	1:F:480:GLN:HE22	1.81	0.46
1:A:431:ARG:NH2	1:A:535:VAL:O	2.48	0.46
1:B:69:LEU:N	1:B:69:LEU:HD12	2.31	0.46
1:B:138:THR:OG1	1:B:401:ARG:NH1	2.49	0.46
1:C:447:PRO:HG3	5:C:4138:HOH:O	2.16	0.46
1:F:142:ARG:NH2	1:F:147:PRO:HD3	2.31	0.46
1:H:359:SER:HB3	4:H:5008:GOL:H31	1.97	0.46
1:I:163:HIS:C	1:I:163:HIS:CD2	2.87	0.46
1:K:485:ASP:OD1	1:K:487:ARG:CB	2.64	0.46
1:E:336:ILE:HB	1:E:425:LEU:HD21	1.96	0.46
1:G:119:TYR:HA	1:G:120:PRO:HD3	1.76	0.46
1:H:163:HIS:CE1	1:H:363:ALA:HB1	2.51	0.46
1:H:433:SER:HB3	1:H:436:ILE:HG13	1.98	0.46
1:K:163:HIS:C	1:K:163:HIS:CD2	2.89	0.46
1:A:64:GLU:OE2	1:I:64:GLU:OE2	2.34	0.46
1:B:193:HIS:NE2	1:B:532:ASP:OD2	2.44	0.46
1:G:431:ARG:HA	1:G:534:GLN:HE22	1.81	0.46
1:L:318:ASN:HB3	1:L:357:VAL:CG1	2.46	0.46
1:B:336:ILE:HB	1:B:425:LEU:HD21	1.97	0.46
1:D:602:HIS:HB3	1:D:614:MET:HA	1.97	0.46
1:E:157:TRP:CE2	1:E:178:ALA:HB3	2.51	0.46
1:C:601:TYR:CE2	1:C:615:ARG:HB2	2.51	0.46
1:J:271:ASN:O	1:J:274:THR:O	2.34	0.46
1:A:436:ILE:HG13	1:A:437:PRO:HD2	1.98	0.45
1:B:554:ARG:HG2	1:B:554:ARG:NH1	2.31	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:255:ARG:HG3	1:F:255:ARG:HH11	1.81	0.45
1:F:465:VAL:O	1:F:466:GLU:HG3	2.16	0.45
1:K:473:VAL:HB	1:K:474:PRO:HA	1.98	0.45
1:C:139:GLU:O	1:C:263:LYS:NZ	2.48	0.45
1:G:487:ARG:HB2	1:G:487:ARG:CZ	2.46	0.45
1:H:382:LEU:HD12	1:H:382:LEU:HA	1.62	0.45
1:I:124:VAL:CG1	1:I:142:ARG:HG2	2.46	0.45
1:J:579:GLN:HG3	5:J:688:HOH:O	2.16	0.45
1:L:337:GLY:N	1:L:367:ASP:HB3	2.30	0.45
1:A:620:MET:HG2	1:I:157:TRP:CH2	2.52	0.45
1:E:379:ARG:NH2	5:E:1663:HOH:O	2.49	0.45
1:H:388:GLY:HA3	5:H:2013:HOH:O	2.15	0.45
1:L:578:PHE:HB3	5:L:1257:HOH:O	2.16	0.45
1:D:205:MET:O	1:D:206:ASN:HB2	2.17	0.45
1:F:334:HIS:HE1	5:F:1640:HOH:O	2.00	0.45
1:A:484:ALA:C	1:A:486:GLY:H	2.20	0.45
1:F:466:GLU:N	5:F:1806:HOH:O	2.49	0.45
1:H:85:MET:HB3	1:H:214:ALA:O	2.16	0.45
1:K:219:THR:HG22	1:K:220:TYR:N	2.29	0.45
1:L:339:ASP:HB2	1:L:575:LYS:HA	1.97	0.45
1:L:446:THR:HG21	1:L:460:TRP:CE2	2.51	0.45
1:B:162:LEU:HG	1:B:165:ALA:HB2	1.98	0.45
1:D:64:GLU:OE2	1:L:64:GLU:OE2	2.35	0.45
1:D:237:ARG:HD3	5:D:2130:HOH:O	2.16	0.45
1:F:197:GLN:O	1:F:365:ARG:CD	2.65	0.45
1:L:69:LEU:HD12	1:L:69:LEU:H	1.81	0.45
1:C:375:LEU:HD13	1:C:380:LEU:HD11	1.99	0.45
1:E:138:THR:HG22	1:E:401:ARG:NE	2.31	0.45
1:G:337:GLY:CA	1:G:367:ASP:HB3	2.46	0.45
1:K:334:HIS:HE1	5:K:672:HOH:O	2.00	0.45
1:A:138:THR:O	1:A:401:ARG:HD2	2.17	0.45
1:C:382:LEU:HD12	1:C:382:LEU:HA	1.80	0.45
1:D:259:ARG:HD2	5:D:1433:HOH:O	2.16	0.45
1:J:325:ASP:O	1:J:326:ASP:HB2	2.16	0.45
5:J:654:HOH:O	1:K:423:GLU:HG2	2.17	0.45
1:K:627:PHE:O	1:K:628:ASP:HB3	2.17	0.45
1:J:175:ALA:HB3	1:J:205:MET:CE	2.47	0.44
1:L:205:MET:HE3	1:L:498:PHE:CE1	2.52	0.44
1:B:535:VAL:HG13	1:B:586:LEU:HD11	1.99	0.44
1:C:404:GLU:CD	1:C:404:GLU:H	2.21	0.44
1:I:379:ARG:HD2	5:I:4231:HOH:O	2.17	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:ARG:HH11	1:H:63:ARG:HH21	1.65	0.44
1:C:397:LEU:HB2	5:C:1942:HOH:O	2.16	0.44
1:I:250:THR:HA	1:I:255:ARG:O	2.17	0.44
1:K:199:TRP:HB2	1:K:218:GLY:O	2.18	0.44
1:A:148:ASN:OD1	1:A:148:ASN:C	2.56	0.44
1:A:599:PHE:O	1:A:616:PRO:HA	2.18	0.44
1:E:70:ARG:HD2	5:E:2588:HOH:O	2.17	0.44
1:E:482:THR:HG1	1:E:488:THR:HG1	1.64	0.44
1:I:538:ARG:HH11	1:I:584:GLN:HE22	1.66	0.44
1:J:465:VAL:CG1	1:J:466:GLU:N	2.81	0.44
1:A:362:PRO:O	1:A:363:ALA:HB3	2.16	0.44
1:A:531:ALA:HB3	1:A:533:PHE:CE1	2.53	0.44
1:D:339:ASP:HB2	1:D:575:LYS:HA	1.98	0.44
1:D:432:MET:H	1:D:534:GLN:HE22	1.63	0.44
1:E:443:ILE:CD1	1:E:504:PHE:HZ	2.31	0.44
1:F:591:LYS:HE2	1:F:593:ASP:OD1	2.18	0.44
1:L:334:HIS:HE1	5:L:684:HOH:O	2.00	0.44
1:A:159:VAL:O	1:A:202:ASP:HA	2.18	0.44
1:A:338:SER:O	1:A:339:ASP:C	2.56	0.44
1:L:545:GLY:CA	1:L:555:THR:HG23	2.47	0.44
1:A:504:PHE:N	1:A:504:PHE:CD1	2.85	0.44
1:B:431:ARG:NE	1:B:534:GLN:NE2	2.65	0.44
1:C:536:LEU:HD11	1:C:589:MET:HE2	1.98	0.44
1:D:63:ARG:NH1	1:L:63:ARG:HH11	2.13	0.44
1:H:370:VAL:HG11	1:H:372:PHE:CZ	2.53	0.44
1:H:472:GLN:O	1:H:473:VAL:HB	2.16	0.44
1:I:271:ASN:ND2	1:I:273:GLU:H	2.15	0.44
1:I:566:PRO:HA	5:I:3613:HOH:O	2.18	0.44
1:J:316:ILE:HD11	1:J:523:LEU:HD22	1.99	0.44
1:A:545:GLY:HA2	1:A:555:THR:HG23	2.00	0.44
1:F:537:GLY:HA2	1:F:567:LEU:HD21	2.00	0.44
1:G:141:GLY:O	1:G:263:LYS:HE3	2.18	0.44
1:H:620:MET:SD	1:H:625:LEU:HD12	2.57	0.44
1:I:446:THR:HG21	1:I:460:TRP:CE2	2.52	0.44
1:I:456:HIS:CE1	1:I:611:MET:HE2	2.51	0.44
1:I:533:PHE:HB2	1:I:578:PHE:CZ	2.53	0.44
1:J:548:LEU:N	1:J:548:LEU:HD23	2.33	0.44
1:H:271:ASN:HD22	1:H:274:THR:H	1.66	0.43
1:A:443:ILE:HD13	1:A:443:ILE:N	2.33	0.43
1:B:176:ASP:OD2	1:H:598:ARG:HD2	2.18	0.43
1:G:88:TYR:CD2	1:G:200:TYR:HE1	2.36	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:559:LEU:O	1:I:561:PRO:HD3	2.17	0.43
1:J:271:ASN:HD22	1:J:274:THR:H	1.66	0.43
1:K:322:ILE:HD12	1:K:326:ASP:HA	2.00	0.43
1:L:255:ARG:HG3	1:L:255:ARG:HH11	1.83	0.43
1:E:498:PHE:HA	1:E:614:MET:O	2.19	0.43
1:L:535:VAL:HG13	1:L:586:LEU:HD11	1.99	0.43
1:B:472:GLN:C	1:B:473:VAL:O	2.56	0.43
1:L:205:MET:CE	1:L:498:PHE:CE1	3.00	0.43
1:A:255:ARG:HG3	1:A:255:ARG:NH1	2.33	0.43
1:C:163:HIS:C	1:C:163:HIS:CD2	2.91	0.43
1:K:447:PRO:HG2	1:K:548:LEU:HD11	2.00	0.43
1:I:536:LEU:HD11	1:I:589:MET:HB2	2.01	0.43
1:A:54:LEU:HD11	5:A:4289:HOH:O	2.18	0.43
1:B:177:ASN:HD22	1:H:597:GLY:CA	2.32	0.43
1:B:430:ARG:CZ	5:B:3569:HOH:O	2.67	0.43
1:D:431:ARG:HA	1:D:534:GLN:HE22	1.84	0.43
1:E:582:GLY:O	1:E:584:GLN:N	2.52	0.43
1:K:498:PHE:HA	1:K:614:MET:O	2.19	0.43
1:L:250:THR:HA	1:L:255:ARG:O	2.18	0.43
1:B:464:GLU:OE2	1:B:489:LYS:HE2	2.19	0.43
1:G:582:GLY:O	1:G:583:PRO:C	2.56	0.43
1:I:255:ARG:NE	1:J:423:GLU:OE1	2.51	0.43
1:J:250:THR:HA	1:J:255:ARG:O	2.17	0.43
1:K:267:VAL:O	1:K:267:VAL:HG22	2.19	0.43
1:L:142:ARG:HD2	1:L:249:ASP:OD2	2.19	0.43
1:L:194:GLN:NE2	5:L:1236:HOH:O	2.52	0.43
1:D:177:ASN:ND2	1:L:598:ARG:H	2.12	0.43
1:D:230:LEU:HD21	1:D:425:LEU:HD22	2.00	0.43
1:E:602:HIS:HB3	1:E:614:MET:HG3	2.01	0.43
1:F:177:ASN:HD22	1:J:597:GLY:CA	2.31	0.43
1:H:314:ALA:HA	1:H:605:LEU:HD22	2.01	0.43
1:I:475:ALA:H	1:I:550:LEU:HD21	1.84	0.43
1:B:197:GLN:O	1:B:365:ARG:HD2	2.18	0.43
1:D:418:SER:O	1:D:419:PHE:C	2.57	0.43
1:F:602:HIS:HB3	1:F:614:MET:HA	2.01	0.43
1:I:252:GLU:HG3	5:I:2806:HOH:O	2.18	0.43
1:A:147:PRO:O	1:A:149:LYS:CE	2.64	0.42
1:A:176:ASP:O	1:I:597:GLY:HA2	2.19	0.42
1:C:281:PRO:HA	1:C:607:GLU:HG2	2.00	0.42
1:D:199:TRP:HA	1:D:219:THR:HA	2.00	0.42
1:I:574:HIS:CD2	5:I:1319:HOH:O	2.72	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:142:ARG:HD3	1:J:249:ASP:OD1	2.19	0.42
1:J:531:ALA:HB3	1:J:533:PHE:CE1	2.54	0.42
1:A:379:ARG:HG2	1:A:409:ARG:HG2	2.01	0.42
1:A:485:ASP:OD2	1:A:487:ARG:HG2	2.19	0.42
1:D:112:ARG:HD3	5:D:984:HOH:O	2.18	0.42
1:H:591:LYS:HE3	1:H:593:ASP:OD1	2.19	0.42
1:I:101:ARG:HG3	1:I:193:HIS:O	2.18	0.42
1:I:268:GLN:NE2	1:I:272:PRO:HD3	2.33	0.42
1:D:271:ASN:ND2	1:D:273:GLU:H	2.17	0.42
1:F:119:TYR:HA	1:F:120:PRO:HD3	1.90	0.42
1:G:433:SER:OG	1:G:435:ASP:HB2	2.19	0.42
1:J:118:GLU:HB3	5:J:2503:HOH:O	2.19	0.42
1:J:560:ASP:C	1:J:562:ASP:H	2.21	0.42
5:K:1301:HOH:O	1:L:423:GLU:HG2	2.18	0.42
1:B:64:GLU:OE2	1:H:64:GLU:OE2	2.37	0.42
1:B:68:ALA:HB1	1:B:112:ARG:HG3	2.02	0.42
1:E:255:ARG:HH11	1:E:255:ARG:CG	2.33	0.42
1:G:536:LEU:HD11	1:G:589:MET:HB2	2.01	0.42
1:A:83:THR:HG23	1:A:258:GLY:O	2.18	0.42
1:C:431:ARG:HA	1:C:534:GLN:HE22	1.85	0.42
1:F:404:GLU:CD	1:F:404:GLU:H	2.23	0.42
1:H:581:PRO:HG2	1:H:584:GLN:OE1	2.19	0.42
1:I:37:ALA:N	5:I:1486:HOH:O	2.52	0.42
1:I:523:LEU:HD23	1:I:523:LEU:C	2.40	0.42
1:L:159:VAL:HB	1:L:178:ALA:HA	2.01	0.42
1:L:560:ASP:HA	1:L:561:PRO:HD3	1.90	0.42
1:A:520:SER:O	1:A:582:GLY:HA3	2.19	0.42
1:D:177:ASN:ND2	1:L:597:GLY:CA	2.82	0.42
1:F:417:ASP:HB2	5:F:3791:HOH:O	2.19	0.42
1:G:492:ARG:NH1	1:G:492:ARG:HG3	2.34	0.42
1:H:536:LEU:HD11	1:H:589:MET:HE3	2.02	0.42
1:I:403:PRO:HB3	5:I:2701:HOH:O	2.18	0.42
1:I:584:GLN:HG2	1:I:585:GLY:N	2.34	0.42
1:J:284:GLY:HA2	1:J:285:PRO:HD3	1.87	0.42
1:A:244:ALA:HA	1:A:312:SER:OG	2.20	0.42
1:A:598:ARG:NH2	5:A:2528:HOH:O	2.42	0.42
1:G:498:PHE:HA	1:G:614:MET:O	2.20	0.42
1:H:245:ASP:HA	1:H:286:TYR:O	2.19	0.42
1:I:382:LEU:HA	1:I:382:LEU:HD12	1.81	0.42
1:K:142:ARG:HE	1:K:147:PRO:HD3	1.84	0.42
1:I:461:GLU:OE1	1:I:503:GLY:HA3	2.19	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:443:ILE:HG23	1:J:459:ILE:HG23	2.01	0.42
1:L:119:TYR:HA	1:L:120:PRO:HD3	1.81	0.42
1:B:157:TRP:CE2	1:B:178:ALA:HB3	2.54	0.42
1:G:401:ARG:HG3	1:G:401:ARG:HH11	1.85	0.42
1:I:506:ILE:O	1:I:619:VAL:HA	2.19	0.42
1:K:285:PRO:HG2	1:K:286:TYR:CE1	2.55	0.42
1:K:434:HIS:HD2	1:K:589:MET:HE1	1.85	0.42
1:L:375:LEU:O	1:L:410:VAL:HB	2.20	0.42
1:B:159:VAL:HB	1:B:178:ALA:HA	2.01	0.42
1:C:276:LYS:HB2	1:C:277:PRO:CD	2.50	0.42
1:D:431:ARG:HH22	1:D:572:LEU:HB3	1.85	0.42
1:F:352:ASP:HB2	5:F:1612:HOH:O	2.20	0.42
1:G:362:PRO:O	1:G:363:ALA:HB3	2.20	0.42
1:A:176:ASP:OD2	1:I:598:ARG:HD2	2.20	0.41
1:B:80:LEU:HB3	1:B:81:PRO:HD2	2.02	0.41
1:B:124:VAL:HG11	1:B:142:ARG:HG2	2.01	0.41
1:D:492:ARG:HE	1:D:492:ARG:HB2	1.50	0.41
1:I:434:HIS:CD2	1:I:438:HIS:CE1	3.08	0.41
1:K:451:LYS:HD3	1:K:549:ALA:O	2.19	0.41
1:L:280:ILE:HB	1:L:281:PRO:HD2	2.01	0.41
1:F:337:GLY:N	1:F:367:ASP:HB3	2.35	0.41
1:G:159:VAL:O	1:G:202:ASP:HA	2.20	0.41
1:K:379:ARG:HG2	1:K:409:ARG:HG2	2.02	0.41
1:A:382:LEU:HD12	1:A:382:LEU:HA	1.82	0.41
1:C:142:ARG:HD3	1:C:249:ASP:OD2	2.20	0.41
1:F:164:GLY:HA3	1:F:198:TRP:CD1	2.55	0.41
1:A:482:THR:HG1	1:A:488:THR:HG1	1.68	0.41
1:C:82:PRO:HD3	1:D:230:LEU:HD13	2.03	0.41
1:D:598:ARG:H	1:L:177:ASN:ND2	2.14	0.41
1:D:553:THR:OG1	1:D:555:THR:O	2.37	0.41
1:F:271:ASN:HD22	1:F:274:THR:H	1.68	0.41
1:G:602:HIS:HB3	1:G:614:MET:HG3	2.02	0.41
1:J:130:PRO:HA	1:J:131:PRO:HD3	1.96	0.41
1:J:571:GLU:O	1:J:571:GLU:HG3	2.20	0.41
1:L:482:THR:HA	1:L:487:ARG:O	2.21	0.41
1:A:149:LYS:HA	1:A:149:LYS:HD3	1.90	0.41
1:B:536:LEU:HD11	1:B:589:MET:CE	2.50	0.41
1:D:63:ARG:NH1	1:L:63:ARG:NH1	2.66	0.41
1:G:521:PRO:HA	1:G:583:PRO:HD3	2.03	0.41
1:H:209:ARG:NH2	5:H:4371:HOH:O	2.52	0.41
1:H:271:ASN:HD21	1:H:273:GLU:HB2	1.86	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:138:THR:O	1:I:401:ARG:HD2	2.20	0.41
1:K:37:ALA:HB3	1:K:40:GLU:OE1	2.21	0.41
1:A:230:LEU:HD23	1:A:230:LEU:HA	1.93	0.41
1:A:536:LEU:HD11	1:A:589:MET:CE	2.51	0.41
1:C:197:GLN:O	1:C:365:ARG:CD	2.67	0.41
1:E:418:SER:O	1:E:419:PHE:C	2.58	0.41
1:F:597:GLY:HA3	1:J:177:ASN:ND2	2.35	0.41
1:H:237:ARG:HD2	1:H:304:TYR:CZ	2.55	0.41
1:L:163:HIS:HE2	1:L:577:VAL:HG23	1.86	0.41
1:L:255:ARG:HG3	1:L:255:ARG:NH1	2.35	0.41
1:C:177:ASN:HD22	1:G:597:GLY:HA3	1.85	0.41
1:E:177:ASN:ND2	1:K:598:ARG:H	2.16	0.41
1:J:174:TRP:CD1	1:J:176:ASP:HB2	2.55	0.41
1:K:587:ARG:HH11	1:K:587:ARG:HD2	1.75	0.41
1:L:142:ARG:HH21	1:L:147:PRO:HD3	1.86	0.41
1:A:303:TRP:CZ3	1:A:371:ASP:HB2	2.56	0.41
1:B:372:PHE:HE1	1:B:380:LEU:HD12	1.86	0.41
1:B:627:PHE:O	1:B:628:ASP:CB	2.67	0.41
1:C:205:MET:HE3	1:C:498:PHE:CE1	2.56	0.41
1:C:536:LEU:CD1	1:C:589:MET:CE	2.95	0.41
1:C:605:LEU:HD12	1:C:608:HIS:CE1	2.56	0.41
1:D:443:ILE:CD1	1:D:504:PHE:HZ	2.34	0.41
1:E:86:TRP:CD2	1:E:113:ILE:HD13	2.56	0.41
1:F:582:GLY:O	1:F:583:PRO:C	2.58	0.41
1:G:325:ASP:O	1:G:326:ASP:HB2	2.21	0.41
1:I:445:LEU:HB2	1:I:518:ASN:HA	2.02	0.41
1:K:76:LEU:HD23	1:K:76:LEU:HA	1.93	0.41
1:K:138:THR:HG21	1:K:401:ARG:NH2	2.35	0.41
1:K:413:THR:CG2	1:K:414:CYS:N	2.84	0.41
1:D:375:LEU:HD13	1:D:380:LEU:HD11	2.02	0.41
1:F:271:ASN:ND2	1:F:273:GLU:H	2.19	0.41
1:I:194:GLN:NE2	5:I:3156:HOH:O	2.52	0.41
1:J:142:ARG:HD2	1:J:249:ASP:OD2	2.21	0.41
1:E:520:SER:O	1:E:582:GLY:CA	2.66	0.40
1:F:142:ARG:HD3	1:F:249:ASP:OD2	2.21	0.40
1:H:520:SER:O	1:H:582:GLY:HA3	2.22	0.40
1:L:504:PHE:CD1	1:L:504:PHE:N	2.88	0.40
1:B:250:THR:HA	1:B:255:ARG:O	2.21	0.40
1:C:142:ARG:HD3	1:C:249:ASP:OD1	2.20	0.40
1:D:157:TRP:CE2	1:D:178:ALA:HB3	2.56	0.40
1:F:533:PHE:HB2	1:F:578:PHE:HZ	1.86	0.40

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:130:PRO:HA	1:G:131:PRO:HD3	1.79	0.40
1:G:620:MET:HE2	1:G:624:ALA:CB	2.51	0.40
1:I:352:ASP:OD2	1:I:353:ASP:N	2.55	0.40
1:K:124:VAL:HG11	1:K:142:ARG:HG2	2.02	0.40
1:L:237:ARG:HD2	1:L:304:TYR:CZ	2.56	0.40
1:L:538:ARG:HH11	1:L:584:GLN:HE22	1.69	0.40
1:C:443:ILE:HD11	1:C:504:PHE:HE2	1.84	0.40
1:C:559:LEU:O	1:C:561:PRO:HD3	2.20	0.40
1:E:597:GLY:CA	1:K:177:ASN:HD22	2.34	0.40
1:F:581:PRO:C	1:F:582:GLY:O	2.60	0.40
1:G:271:ASN:O	1:G:274:THR:O	2.39	0.40
1:K:209:ARG:NH1	1:K:610:ASP:CB	2.84	0.40
1:D:304:TYR:HB2	1:D:370:VAL:HG23	2.03	0.40
1:E:285:PRO:HG2	1:E:286:TYR:CE1	2.56	0.40
1:E:581:PRO:C	1:E:582:GLY:O	2.59	0.40
1:F:43:PRO:HB3	1:F:404:GLU:HG3	2.03	0.40
1:H:575:LYS:HB2	1:H:578:PHE:HE1	1.86	0.40
1:K:325:ASP:O	1:K:326:ASP:HB2	2.21	0.40
1:K:513:GLN:NE2	1:K:536:LEU:HD12	2.32	0.40
1:K:570:ASN:OD1	4:K:5011:GOL:H32	2.21	0.40
1:A:598:ARG:HD2	1:I:176:ASP:OD2	2.22	0.40
1:B:86:TRP:CD2	1:B:113:ILE:HD13	2.56	0.40
1:C:401:ARG:HD3	5:C:2373:HOH:O	2.22	0.40
1:D:431:ARG:NH2	1:D:572:LEU:O	2.55	0.40
1:F:175:ALA:HB3	1:F:205:MET:HE2	2.03	0.40
1:K:76:LEU:HB3	1:K:293:ILE:HD12	2.03	0.40
1:K:352:ASP:CG	1:K:353:ASP:H	2.24	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	583/612 (95%)	558 (96%)	23 (4%)	2 (0%)	41	50
1	B	583/612 (95%)	560 (96%)	22 (4%)	1 (0%)	47	58
1	C	583/612 (95%)	557 (96%)	26 (4%)	0	100	100
1	D	583/612 (95%)	561 (96%)	22 (4%)	0	100	100
1	E	583/612 (95%)	558 (96%)	23 (4%)	2 (0%)	41	50
1	F	583/612 (95%)	556 (95%)	24 (4%)	3 (0%)	29	35
1	G	583/612 (95%)	556 (95%)	24 (4%)	3 (0%)	29	35
1	H	583/612 (95%)	564 (97%)	18 (3%)	1 (0%)	47	58
1	I	583/612 (95%)	546 (94%)	34 (6%)	3 (0%)	29	35
1	J	583/612 (95%)	552 (95%)	29 (5%)	2 (0%)	41	50
1	K	583/612 (95%)	560 (96%)	23 (4%)	0	100	100
1	L	583/612 (95%)	558 (96%)	25 (4%)	0	100	100
All	All	6996/7344 (95%)	6686 (96%)	293 (4%)	17 (0%)	47	58

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	582	GLY
1	G	555	THR
1	G	556	PRO
1	G	583	PRO
1	H	473	VAL
1	A	473	VAL
1	A	485	ASP
1	F	582	GLY
1	F	583	PRO
1	I	582	GLY
1	J	582	GLY
1	J	583	PRO
1	E	583	PRO
1	B	473	VAL
1	F	484	ALA
1	I	583	PRO
1	I	501	GLY

### 5.3.2 Protein sidechains [i](#)

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	484/499 (97%)	482 (100%)	2 (0%)	91	96
1	B	484/499 (97%)	482 (100%)	2 (0%)	91	96
1	C	484/499 (97%)	483 (100%)	1 (0%)	93	97
1	D	484/499 (97%)	483 (100%)	1 (0%)	93	97
1	E	484/499 (97%)	483 (100%)	1 (0%)	93	97
1	F	484/499 (97%)	483 (100%)	1 (0%)	93	97
1	G	484/499 (97%)	480 (99%)	4 (1%)	81	91
1	H	484/499 (97%)	483 (100%)	1 (0%)	93	97
1	I	484/499 (97%)	481 (99%)	3 (1%)	86	94
1	J	484/499 (97%)	481 (99%)	3 (1%)	86	94
1	K	484/499 (97%)	482 (100%)	2 (0%)	91	96
1	L	484/499 (97%)	478 (99%)	6 (1%)	71	84
All	All	5808/5988 (97%)	5781 (100%)	27 (0%)	88	95

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	397	LEU
1	A	578	PHE
1	B	418	SER
1	B	473	VAL
1	C	353	ASP
1	D	230	LEU
1	E	418	SER
1	F	473	VAL
1	G	445	LEU
1	G	487	ARG
1	G	548	LEU
1	G	578	PHE
1	H	472	GLN
1	I	138	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	I	476	GLU
1	I	558	ARG
1	J	466	GLU
1	J	472	GLN
1	J	578	PHE
1	K	138	THR
1	K	149	LYS
1	L	128	LEU
1	L	354	THR
1	L	431	ARG
1	L	558	ARG
1	L	561	PRO
1	L	578	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (108) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
1	A	177	ASN
1	A	191	ASN
1	A	271	ASN
1	A	334	HIS
1	A	499	ASN
1	A	513	GLN
1	A	534	GLN
1	B	91	GLN
1	B	177	ASN
1	B	191	ASN
1	B	271	ASN
1	B	318	ASN
1	B	334	HIS
1	B	456	HIS
1	B	499	ASN
1	B	513	GLN
1	B	534	GLN
1	B	574	HIS
1	B	584	GLN
1	C	91	GLN
1	C	177	ASN
1	C	191	ASN
1	C	271	ASN
1	C	318	ASN

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	334	HIS
1	C	499	ASN
1	C	534	GLN
1	D	177	ASN
1	D	191	ASN
1	D	271	ASN
1	D	334	HIS
1	D	499	ASN
1	D	513	GLN
1	D	534	GLN
1	D	584	GLN
1	E	91	GLN
1	E	177	ASN
1	E	191	ASN
1	E	271	ASN
1	E	318	ASN
1	E	334	HIS
1	E	456	HIS
1	E	472	GLN
1	E	534	GLN
1	E	584	GLN
1	F	177	ASN
1	F	191	ASN
1	F	271	ASN
1	F	334	HIS
1	F	456	HIS
1	F	513	GLN
1	F	534	GLN
1	G	177	ASN
1	G	191	ASN
1	G	271	ASN
1	G	318	ASN
1	G	334	HIS
1	G	534	GLN
1	G	574	HIS
1	G	584	GLN
1	H	177	ASN
1	H	191	ASN
1	H	271	ASN
1	H	318	ASN
1	H	334	HIS
1	H	472	GLN

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	H	499	ASN
1	H	534	GLN
1	I	177	ASN
1	I	191	ASN
1	I	271	ASN
1	I	334	HIS
1	I	456	HIS
1	I	499	ASN
1	I	513	GLN
1	I	534	GLN
1	I	574	HIS
1	I	584	GLN
1	J	177	ASN
1	J	191	ASN
1	J	271	ASN
1	J	334	HIS
1	J	472	GLN
1	J	499	ASN
1	J	513	GLN
1	J	534	GLN
1	J	584	GLN
1	K	177	ASN
1	K	191	ASN
1	K	197	GLN
1	K	206	ASN
1	K	271	ASN
1	K	334	HIS
1	K	513	GLN
1	K	534	GLN
1	K	584	GLN
1	L	91	GLN
1	L	177	ASN
1	L	191	ASN
1	L	194	GLN
1	L	271	ASN
1	L	318	ASN
1	L	334	HIS
1	L	499	ASN
1	L	513	GLN
1	L	534	GLN
1	L	584	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 60 ligands modelled in this entry, 36 are monoatomic - leaving 24 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	C2O	L	1002	1	0,2,2	-	-	-		
4	GOL	L	5012	-	5,5,5	0.48	0	5,5,5	0.94	0
4	GOL	K	5011	-	5,5,5	0.37	0	5,5,5	1.18	0
4	GOL	D	5004	-	5,5,5	0.41	0	5,5,5	0.80	0
4	GOL	F	5006	-	5,5,5	0.25	0	5,5,5	0.78	0
4	GOL	B	5002	-	5,5,5	0.37	0	5,5,5	0.73	0
3	C2O	H	1002	1	0,2,2	-	-	-		
4	GOL	G	5007	-	5,5,5	0.20	0	5,5,5	0.60	0
3	C2O	J	1002	1	0,2,2	-	-	-		
3	C2O	G	1002	1	0,2,2	-	-	-		
4	GOL	E	5005	-	5,5,5	0.37	0	5,5,5	0.70	0
3	C2O	D	1002	1	0,2,2	-	-	-		
3	C2O	A	1002	1	0,2,2	-	-	-		
3	C2O	F	1002	1	0,2,2	-	-	-		
4	GOL	H	5008	-	5,5,5	0.38	0	5,5,5	0.78	0
4	GOL	J	5010	-	5,5,5	0.28	0	5,5,5	0.54	0
4	GOL	I	5009	-	5,5,5	0.27	0	5,5,5	0.89	0
3	C2O	I	1002	1	0,2,2	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	GOL	C	5003	-	5,5,5	0.48	0	5,5,5	1.06	0
3	C2O	C	1002	1	0,2,2	-	-	-	-	-
4	GOL	A	5001	-	5,5,5	0.45	0	5,5,5	0.94	0
3	C2O	E	1002	1	0,2,2	-	-	-	-	-
3	C2O	B	1002	1	0,2,2	-	-	-	-	-
3	C2O	K	1002	1	0,2,2	-	-	-	-	-

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	E	5005	-	-	4/4/4/4	-
4	GOL	I	5009	-	-	2/4/4/4	-
4	GOL	B	5002	-	-	2/4/4/4	-
4	GOL	G	5007	-	-	3/4/4/4	-
4	GOL	L	5012	-	-	2/4/4/4	-
4	GOL	K	5011	-	-	0/4/4/4	-
4	GOL	C	5003	-	-	2/4/4/4	-
4	GOL	H	5008	-	-	3/4/4/4	-
4	GOL	D	5004	-	-	0/4/4/4	-
4	GOL	J	5010	-	-	2/4/4/4	-
4	GOL	F	5006	-	-	4/4/4/4	-
4	GOL	A	5001	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	5002	GOL	O2-C2-C3-O3
4	C	5003	GOL	O1-C1-C2-C3
4	G	5007	GOL	O1-C1-C2-C3
4	E	5005	GOL	O1-C1-C2-O2
4	F	5006	GOL	O2-C2-C3-O3
4	A	5001	GOL	O1-C1-C2-C3

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
4	A	5001	GOL	C1-C2-C3-O3
4	B	5002	GOL	C1-C2-C3-O3
4	E	5005	GOL	O1-C1-C2-C3
4	E	5005	GOL	C1-C2-C3-O3
4	F	5006	GOL	O1-C1-C2-C3
4	F	5006	GOL	C1-C2-C3-O3
4	H	5008	GOL	O1-C1-C2-C3
4	H	5008	GOL	C1-C2-C3-O3
4	I	5009	GOL	O1-C1-C2-C3
4	J	5010	GOL	O1-C1-C2-C3
4	L	5012	GOL	O1-C1-C2-C3
4	A	5001	GOL	O1-C1-C2-O2
4	C	5003	GOL	O1-C1-C2-O2
4	G	5007	GOL	O1-C1-C2-O2
4	H	5008	GOL	O1-C1-C2-O2
4	J	5010	GOL	O1-C1-C2-O2
4	E	5005	GOL	O2-C2-C3-O3
4	A	5001	GOL	O2-C2-C3-O3
4	L	5012	GOL	O1-C1-C2-O2
4	F	5006	GOL	O1-C1-C2-O2
4	G	5007	GOL	C1-C2-C3-O3
4	I	5009	GOL	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	K	5011	GOL	2	0
4	D	5004	GOL	1	0
4	H	5008	GOL	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	587/612 (95%)	-0.31	31 (5%) 26 33	15, 26, 51, 68	2 (0%)
1	B	587/612 (95%)	-0.32	21 (3%) 42 49	14, 25, 47, 69	4 (0%)
1	C	587/612 (95%)	-0.43	18 (3%) 49 56	14, 22, 46, 67	0
1	D	587/612 (95%)	-0.47	10 (1%) 70 76	14, 22, 44, 66	0
1	E	587/612 (95%)	-0.38	24 (4%) 37 44	14, 23, 47, 71	1 (0%)
1	F	587/612 (95%)	-0.32	24 (4%) 37 44	14, 23, 47, 69	3 (0%)
1	G	587/612 (95%)	-0.38	27 (4%) 32 39	14, 24, 47, 70	1 (0%)
1	H	587/612 (95%)	-0.38	20 (3%) 45 52	15, 24, 45, 70	2 (0%)
1	I	587/612 (95%)	-0.18	32 (5%) 25 31	15, 25, 53, 74	2 (0%)
1	J	587/612 (95%)	-0.39	16 (2%) 54 62	15, 23, 45, 61	2 (0%)
1	K	587/612 (95%)	-0.32	25 (4%) 35 42	15, 25, 49, 68	1 (0%)
1	L	587/612 (95%)	-0.32	23 (3%) 39 46	16, 25, 50, 71	1 (0%)
All	All	7044/7344 (95%)	-0.35	271 (3%) 40 47	14, 24, 48, 74	19 (0%)

All (271) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	472	GLN	31.7
1	L	472	GLN	21.9
1	H	473	VAL	17.4
1	I	473	VAL	17.0
1	F	472	GLN	16.8
1	B	472	GLN	16.8
1	F	473	VAL	15.7
1	K	473	VAL	12.2
1	H	472	GLN	12.0
1	J	472	GLN	11.9
1	A	472	GLN	11.5

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	473	VAL	11.0
1	E	472	GLN	10.3
1	L	38	PRO	7.4
1	D	38	PRO	6.5
1	C	38	PRO	6.3
1	J	38	PRO	5.8
1	H	414	CYS	5.6
1	B	414	CYS	5.6
1	F	414	CYS	5.5
1	L	37	ALA	5.5
1	E	38	PRO	5.5
1	G	414	CYS	5.3
1	G	416	GLU	5.2
1	L	416	GLU	5.2
1	I	38	PRO	5.1
1	K	414	CYS	5.1
1	L	563	THR	5.0
1	E	487	ARG	5.0
1	H	37	ALA	5.0
1	H	38	PRO	4.9
1	K	38	PRO	4.8
1	I	37	ALA	4.8
1	A	37	ALA	4.7
1	K	131	PRO	4.7
1	I	484	ALA	4.7
1	G	37	ALA	4.6
1	I	416	GLU	4.6
1	C	414	CYS	4.6
1	F	466	GLU	4.6
1	E	414	CYS	4.6
1	A	473	VAL	4.5
1	K	487	ARG	4.5
1	J	131	PRO	4.5
1	A	38	PRO	4.4
1	L	414	CYS	4.4
1	B	37	ALA	4.3
1	J	37	ALA	4.3
1	I	414	CYS	4.3
1	I	275	GLY	4.3
1	C	37	ALA	4.2
1	L	487	ARG	4.2
1	K	37	ALA	4.2

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	F	562	ASP	4.2
1	D	414	CYS	4.2
1	J	414	CYS	4.2
1	L	466	GLU	4.2
1	F	582	GLY	4.2
1	A	414	CYS	4.2
1	C	416	GLU	4.1
1	A	484	ALA	4.1
1	I	487	ARG	4.1
1	D	37	ALA	4.1
1	F	416	GLU	4.1
1	E	582	GLY	3.9
1	A	416	GLU	3.9
1	C	131	PRO	3.9
1	K	353	ASP	3.9
1	H	131	PRO	3.9
1	K	129	GLY	3.9
1	B	487	ARG	3.9
1	A	563	THR	3.8
1	E	466	GLU	3.8
1	B	38	PRO	3.8
1	F	275	GLY	3.8
1	C	59	ASP	3.7
1	J	582	GLY	3.7
1	K	275	GLY	3.7
1	I	354	THR	3.7
1	J	354	THR	3.7
1	A	466	GLU	3.7
1	G	582	GLY	3.7
1	L	415	GLU	3.6
1	H	416	GLU	3.6
1	K	354	THR	3.6
1	G	485	ASP	3.5
1	D	354	THR	3.5
1	G	487	ARG	3.5
1	K	416	GLU	3.5
1	B	131	PRO	3.5
1	G	562	ASP	3.5
1	I	562	ASP	3.5
1	L	562	ASP	3.5
1	G	418	SER	3.4
1	I	485	ASP	3.4

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	416	GLU	3.4
1	E	37	ALA	3.4
1	I	564	PRO	3.4
1	C	466	GLU	3.4
1	B	466	GLU	3.3
1	D	466	GLU	3.3
1	I	466	GLU	3.3
1	D	131	PRO	3.3
1	A	275	GLY	3.3
1	I	465	VAL	3.3
1	E	131	PRO	3.2
1	K	59	ASP	3.2
1	A	562	ASP	3.2
1	B	416	GLU	3.2
1	B	59	ASP	3.2
1	A	487	ARG	3.2
1	L	252	GLU	3.2
1	A	354	THR	3.2
1	F	487	ARG	3.2
1	A	59	ASP	3.2
1	F	37	ALA	3.2
1	C	582	GLY	3.2
1	F	353	ASP	3.2
1	I	353	ASP	3.2
1	F	274	THR	3.1
1	G	252	GLU	3.1
1	B	437	PRO	3.1
1	A	486	GLY	3.1
1	G	353	ASP	3.1
1	A	131	PRO	3.1
1	E	485	ASP	3.0
1	J	275	GLY	3.0
1	K	484	ALA	3.0
1	H	275	GLY	3.0
1	H	354	THR	3.0
1	C	487	ARG	3.0
1	H	418	SER	3.0
1	K	472	GLN	3.0
1	I	563	THR	3.0
1	J	466	GLU	2.9
1	K	582	GLY	2.9
1	H	59	ASP	2.9

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	L	433	SER	2.9
1	C	486	GLY	2.9
1	J	353	ASP	2.9
1	G	132	GLY	2.9
1	F	38	PRO	2.9
1	A	485	ASP	2.8
1	C	564	PRO	2.8
1	B	354	THR	2.8
1	H	274	THR	2.8
1	F	131	PRO	2.8
1	G	466	GLU	2.8
1	L	274	THR	2.8
1	A	418	SER	2.8
1	E	252	GLU	2.8
1	B	562	ASP	2.8
1	D	487	ARG	2.8
1	E	416	GLU	2.8
1	I	475	ALA	2.8
1	I	59	ASP	2.7
1	E	435	ASP	2.7
1	L	564	PRO	2.7
1	J	416	GLU	2.7
1	G	131	PRO	2.7
1	J	562	ASP	2.7
1	F	418	SER	2.6
1	J	561	PRO	2.6
1	I	628	ASP	2.6
1	K	485	ASP	2.6
1	L	353	ASP	2.6
1	F	354	THR	2.6
1	L	39	GLY	2.6
1	G	354	THR	2.6
1	E	563	THR	2.6
1	L	275	GLY	2.6
1	C	353	ASP	2.6
1	E	59	ASP	2.6
1	E	465	VAL	2.6
1	A	433	SER	2.6
1	E	415	GLU	2.6
1	J	418	SER	2.6
1	I	558	ARG	2.6
1	A	465	VAL	2.6

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	E	562	ASP	2.6
1	F	563	THR	2.5
1	L	485	ASP	2.5
1	C	418	SER	2.5
1	L	418	SER	2.5
1	F	252	GLU	2.5
1	I	252	GLU	2.5
1	G	59	ASP	2.5
1	I	561	PRO	2.5
1	E	473	VAL	2.5
1	C	354	THR	2.5
1	F	561	PRO	2.5
1	A	435	ASP	2.5
1	C	562	ASP	2.5
1	B	435	ASP	2.5
1	L	354	THR	2.5
1	E	486	GLY	2.5
1	D	353	ASP	2.5
1	A	146	GLU	2.4
1	K	415	GLU	2.4
1	K	466	GLU	2.4
1	F	486	GLY	2.4
1	B	57	ALA	2.4
1	H	415	GLU	2.4
1	E	561	PRO	2.4
1	D	275	GLY	2.4
1	E	353	ASP	2.4
1	A	564	PRO	2.4
1	K	57	ALA	2.4
1	F	253	ASP	2.3
1	H	132	GLY	2.3
1	L	561	PRO	2.3
1	B	465	VAL	2.3
1	L	473	VAL	2.3
1	F	59	ASP	2.3
1	I	274	THR	2.3
1	I	582	GLY	2.3
1	K	486	GLY	2.3
1	I	133	THR	2.3
1	I	418	SER	2.3
1	K	270	SER	2.3
1	C	485	ASP	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	G	564	PRO	2.3
1	A	270	SER	2.3
1	L	484	ALA	2.3
1	E	354	THR	2.3
1	I	486	GLY	2.3
1	H	353	ASP	2.3
1	F	437	PRO	2.2
1	G	38	PRO	2.2
1	G	563	THR	2.2
1	B	353	ASP	2.2
1	I	437	PRO	2.2
1	A	57	ALA	2.2
1	A	133	THR	2.2
1	G	486	GLY	2.2
1	A	561	PRO	2.2
1	G	472	GLN	2.2
1	K	418	SER	2.2
1	A	39	GLY	2.2
1	E	129	GLY	2.2
1	J	59	ASP	2.2
1	I	550	LEU	2.2
1	H	466	GLU	2.2
1	B	485	ASP	2.2
1	G	63	ARG	2.1
1	G	484	ALA	2.1
1	G	146	GLU	2.1
1	K	562	ASP	2.1
1	F	564	PRO	2.1
1	G	272	PRO	2.1
1	K	130	PRO	2.1
1	B	628	ASP	2.1
1	I	435	ASP	2.1
1	I	272	PRO	2.1
1	H	130	PRO	2.1
1	G	479	ILE	2.1
1	C	628	ASP	2.1
1	H	252	GLU	2.1
1	J	132	GLY	2.1
1	K	39	GLY	2.1
1	B	561	PRO	2.1
1	A	272	PRO	2.1
1	G	628	ASP	2.0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	H	133	THR	2.0
1	B	549	ALA	2.0
1	C	415	GLU	2.0
1	A	274	THR	2.0
1	H	435	ASP	2.0
1	G	275	GLY	2.0
1	A	276	LYS	2.0
1	E	484	ALA	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	GOL	K	5011	6/6	0.84	0.18	29,41,42,43	0
4	GOL	D	5004	6/6	0.85	0.16	34,36,38,38	0
4	GOL	E	5005	6/6	0.86	0.14	35,40,43,43	0
4	GOL	L	5012	6/6	0.86	0.15	34,37,39,39	0
4	GOL	B	5002	6/6	0.88	0.16	33,39,42,42	0
4	GOL	H	5008	6/6	0.89	0.14	26,33,35,36	0
4	GOL	A	5001	6/6	0.89	0.14	25,32,38,39	0
4	GOL	C	5003	6/6	0.89	0.17	26,28,32,34	0
4	GOL	F	5006	6/6	0.91	0.13	38,39,41,43	0
4	GOL	I	5009	6/6	0.92	0.14	28,36,39,40	0
4	GOL	J	5010	6/6	0.93	0.12	27,35,35,37	0
3	C2O	A	1002	3/3	0.93	0.09	41,41,44,52	0
4	GOL	G	5007	6/6	0.93	0.11	30,39,41,42	0
3	C2O	K	1002	3/3	0.94	0.09	42,42,45,46	0
3	C2O	I	1002	3/3	0.95	0.06	37,37,46,47	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	C2O	B	1002	3/3	0.95	0.07	40,40,41,48	0
3	C2O	L	1002	3/3	0.95	0.08	39,39,41,46	0
3	C2O	J	1002	3/3	0.96	0.07	29,29,38,43	0
3	C2O	H	1002	3/3	0.96	0.07	38,38,40,45	0
3	C2O	C	1002	3/3	0.96	0.09	29,29,39,41	0
3	C2O	D	1002	3/3	0.97	0.06	30,30,39,41	0
3	C2O	F	1002	3/3	0.97	0.09	38,38,39,48	0
3	C2O	G	1002	3/3	0.97	0.06	41,41,42,49	0
2	CU	L	1005	1/1	0.97	0.03	41,41,41,41	0
3	C2O	E	1002	3/3	0.98	0.06	32,32,40,40	0
2	CU	K	1005	1/1	0.98	0.02	42,42,42,42	0
2	CU	E	1000	1/1	0.99	0.05	45,45,45,45	0
2	CU	E	1005	1/1	0.99	0.03	42,42,42,42	0
2	CU	F	1005	1/1	0.99	0.03	38,38,38,38	0
2	CU	G	1005	1/1	0.99	0.03	39,39,39,39	0
2	CU	H	1000	1/1	0.99	0.04	49,49,49,49	0
2	CU	H	1004	1/1	0.99	0.03	43,43,43,43	0
2	CU	I	1004	1/1	0.99	0.03	43,43,43,43	0
2	CU	I	1005	1/1	0.99	0.04	42,42,42,42	0
2	CU	J	1000	1/1	0.99	0.02	40,40,40,40	0
2	CU	J	1004	1/1	0.99	0.04	41,41,41,41	0
2	CU	J	1005	1/1	0.99	0.02	39,39,39,39	0
2	CU	K	1000	1/1	0.99	0.03	43,43,43,43	0
2	CU	K	1004	1/1	0.99	0.04	40,40,40,40	0
2	CU	A	1004	1/1	0.99	0.05	41,41,41,41	0
2	CU	L	1004	1/1	0.99	0.03	43,43,43,43	0
2	CU	A	1005	1/1	0.99	0.03	43,43,43,43	0
2	CU	B	1004	1/1	0.99	0.03	40,40,40,40	0
2	CU	C	1005	1/1	0.99	0.03	37,37,37,37	0
2	CU	D	1004	1/1	0.99	0.04	38,38,38,38	0
2	CU	D	1005	1/1	0.99	0.03	38,38,38,38	0
2	CU	G	1004	1/1	1.00	0.04	43,43,43,43	0
2	CU	L	1000	1/1	1.00	0.04	43,43,43,43	0
2	CU	D	1000	1/1	1.00	0.02	37,37,37,37	0
2	CU	A	1000	1/1	1.00	0.04	50,50,50,50	0
2	CU	B	1005	1/1	1.00	0.06	37,37,37,37	0
2	CU	H	1005	1/1	1.00	0.03	36,36,36,36	0
2	CU	I	1000	1/1	1.00	0.02	46,46,46,46	0
2	CU	C	1000	1/1	1.00	0.03	43,43,43,43	0
2	CU	E	1004	1/1	1.00	0.03	41,41,41,41	0
2	CU	C	1004	1/1	1.00	0.05	39,39,39,39	0
2	CU	F	1000	1/1	1.00	0.03	42,42,42,42	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CU	F	1004	1/1	1.00	0.07	42,42,42,42	0
2	CU	B	1000	1/1	1.00	0.03	43,43,43,43	0
2	CU	G	1000	1/1	1.00	0.03	43,43,43,43	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.