



# Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 07:20 am BST

PDB ID : 3PCF  
Title : STRUCTURE OF PROTOCATECHUATE 3,4-DIOXYGENASE COM-  
PLEXED WITH 3-FLURO-4-HYDROXYBENZOATE  
Authors : Orville, A.M.; Elango, N.; Lipscomb, J.D.; Ohlendorf, D.H.  
Deposited on : 1997-06-27  
Resolution : 2.15 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 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

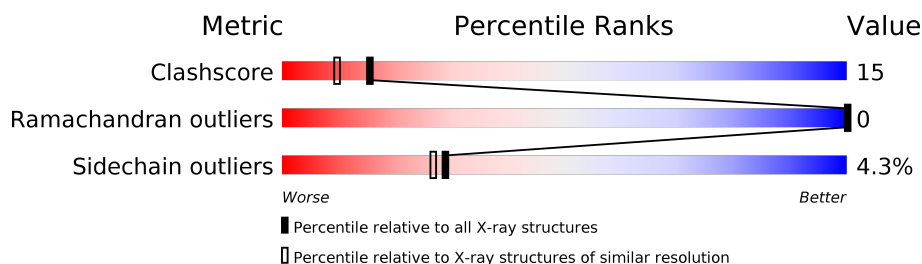
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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))
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	200	 70% 25% 6% .
1	B	200	 69% 27% . .
1	C	200	 67% 28% . .
1	D	200	 70% 24% 6% .
1	E	200	 63% 33% . .
1	F	200	 62% 36% . .
2	M	238	 71% 21% 5% . .
2	N	238	 69% 25% . .

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	O	238	<div><div></div><div>71%23%</div><div></div><div></div></div>
2	P	238	<div><div></div><div>71%23%</div><div></div><div></div></div>
2	Q	238	<div><div></div><div>69%24%</div><div></div><div></div></div>
2	R	238	<div><div></div><div>63%27%6%</div><div></div><div></div></div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 22080 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 PROTOCATECHUATE 3,4-DIOXYGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	200	Total	C	N	O	S	0	0	0
			1571	993	276	299	3			
1	B	200	Total	C	N	O	S	0	0	0
			1571	993	276	299	3			
1	C	200	Total	C	N	O	S	0	0	0
			1571	993	276	299	3			
1	D	200	Total	C	N	O	S	0	0	0
			1571	993	276	299	3			
1	E	200	Total	C	N	O	S	0	0	0
			1571	993	276	299	3			
1	F	200	Total	C	N	O	S	0	0	0
			1571	993	276	299	3			

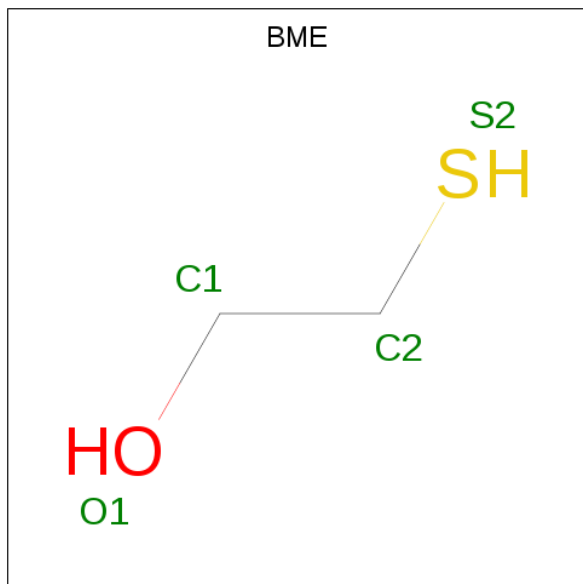
- Molecule 2 is a protein called PROTOCATECHUATE 3,4-DIOXYGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	233	Total	C	N	O	S	0	0	0
			1840	1171	334	328	7			
2	N	233	Total	C	N	O	S	0	0	0
			1840	1171	334	328	7			
2	O	233	Total	C	N	O	S	0	0	0
			1840	1171	334	328	7			
2	P	233	Total	C	N	O	S	0	0	0
			1840	1171	334	328	7			
2	Q	233	Total	C	N	O	S	0	0	0
			1840	1171	334	328	7			
2	R	233	Total	C	N	O	S	0	0	0
			1840	1171	334	328	7			

- Molecule 3 is FE (III) ION (three-letter code: FE) (formula: Fe).

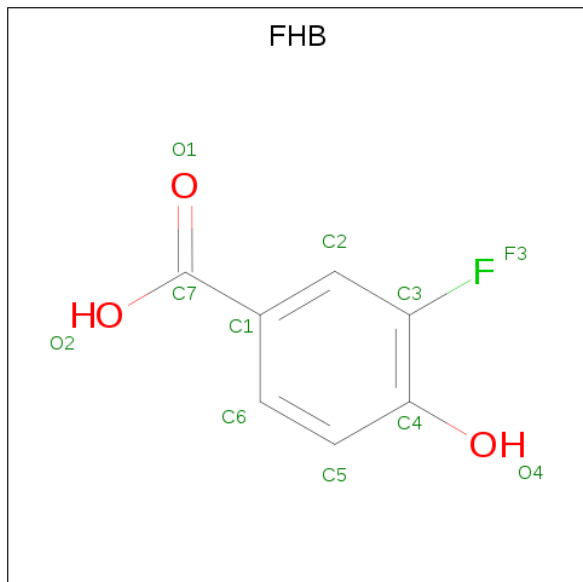
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	P	1	Total Fe 1 1	0	0
3	Q	1	Total Fe 1 1	0	0
3	N	1	Total Fe 1 1	0	0
3	O	1	Total Fe 1 1	0	0
3	R	1	Total Fe 1 1	0	0
3	M	1	Total Fe 1 1	0	0

- Molecule 4 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula:  $C_2H_6OS$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	M	1	Total C O S 4 2 1 1	0	0
4	N	1	Total C O S 4 2 1 1	0	0
4	O	1	Total C O S 4 2 1 1	0	0
4	P	1	Total C O S 4 2 1 1	0	0
4	Q	1	Total C O S 4 2 1 1	0	0
4	R	1	Total C O S 4 2 1 1	0	0

- Molecule 5 is 3-FLUORO-4-HYDROXYBENZOIC ACID (three-letter code: FHB) (formula:  $C_7H_5FO_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	M	1	Total	C	F	O	0	0
			11	7	1	3		
5	M	1	Total	C	F	O	0	0
			11	7	1	3		
5	N	1	Total	C	F	O	0	0
			11	7	1	3		
5	N	1	Total	C	F	O	0	0
			11	7	1	3		
5	O	1	Total	C	F	O	0	0
			11	7	1	3		
5	O	1	Total	C	F	O	0	0
			11	7	1	3		
5	P	1	Total	C	F	O	0	0
			11	7	1	3		
5	P	1	Total	C	F	O	0	0
			11	7	1	3		
5	Q	1	Total	C	F	O	0	0
			11	7	1	3		
5	Q	1	Total	C	F	O	0	0
			11	7	1	3		
5	R	1	Total	C	F	O	0	0
			11	7	1	3		
5	R	1	Total	C	F	O	0	0
			11	7	1	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	85	Total 85	O 85	0	0
6	M	158	Total 158	O 158	0	0
6	B	80	Total 80	O 80	0	0
6	N	166	Total 166	O 166	0	0
6	C	86	Total 86	O 86	0	0
6	O	155	Total 155	O 155	0	0
6	D	80	Total 80	O 80	0	0
6	P	155	Total 155	O 155	0	0
6	E	84	Total 84	O 84	0	0
6	Q	159	Total 159	O 159	0	0
6	F	83	Total 83	O 83	0	0
6	R	161	Total 161	O 161	0	0

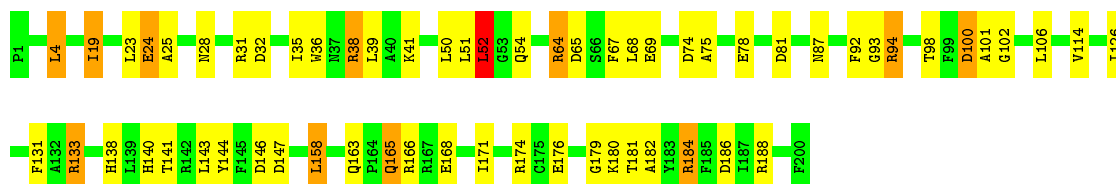
### 3 Residue-property plots [i](#)

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. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

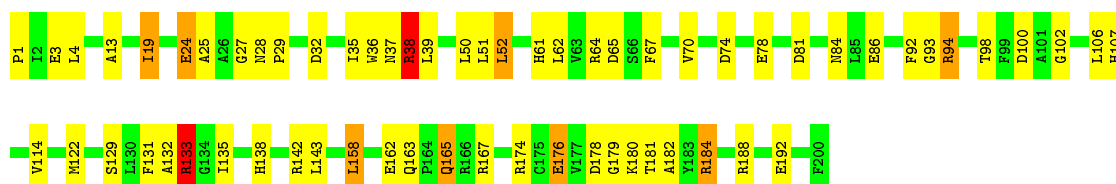
#### • Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain A: 



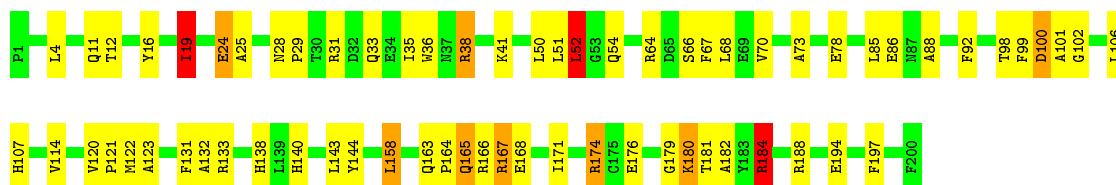
#### • Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain B: 



#### • Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain C: 



#### • Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

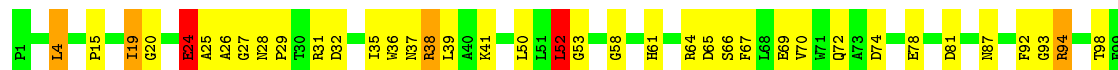
Chain D: 



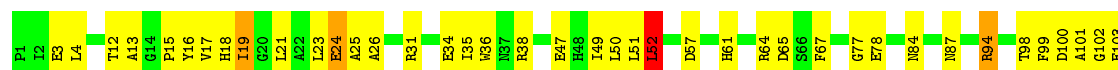




• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE



• Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

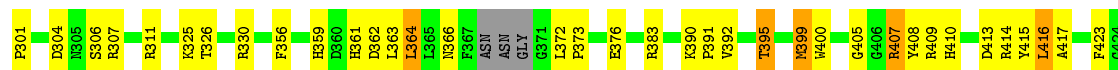


• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE



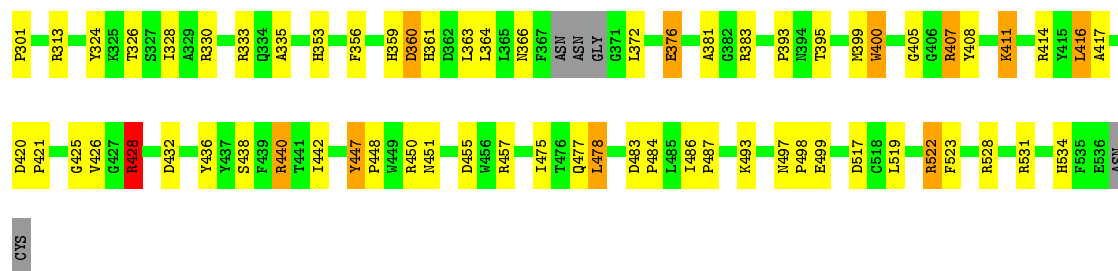
CYS

• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE



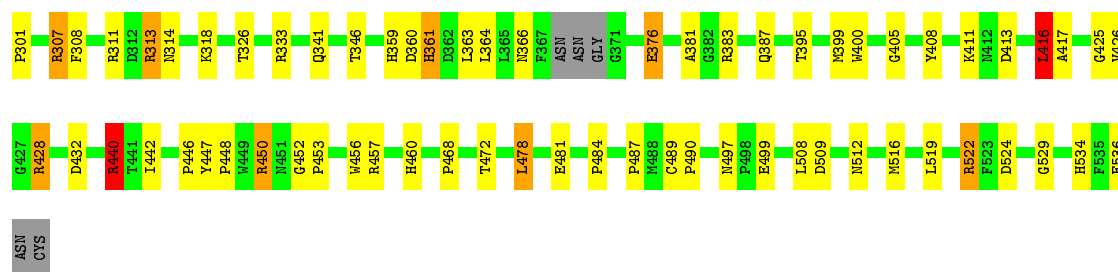
• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE





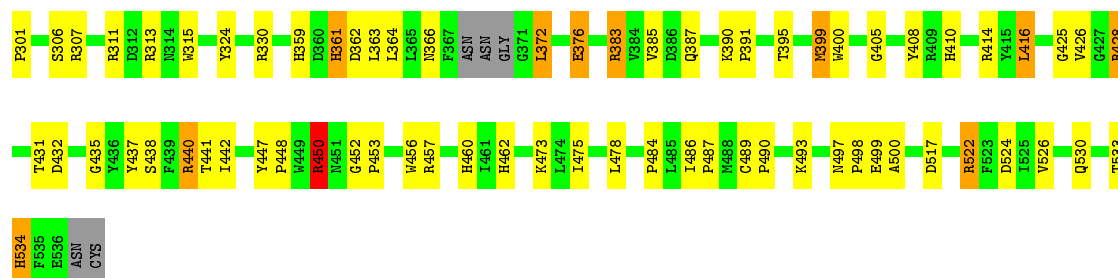
• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain P: 71% 23%



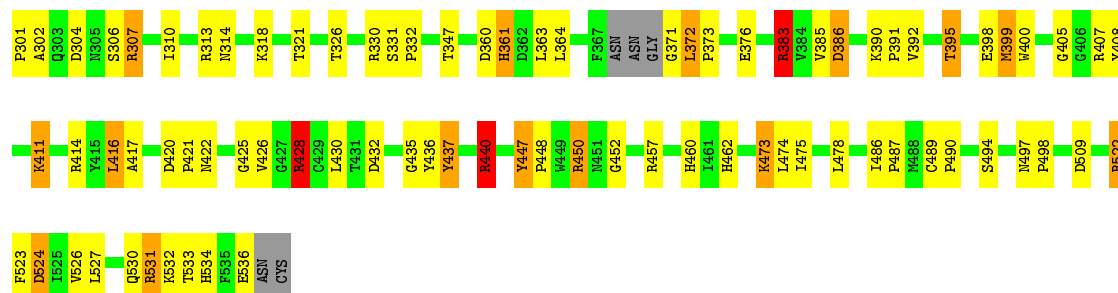
• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain Q: 69% 24%



• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain R: 63% 27% 6%



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	196.03Å 127.22Å 133.70Å 90.00° 97.70° 90.00°	Depositor
Resolution (Å)	6.00 – 2.15	Depositor
% Data completeness (in resolution range)	93.3 (6.00-2.15)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.179 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	22080	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FHB, FE, BME

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	1.01	1/1611 (0.1%)	1.77	35/2195 (1.6%)
1	B	1.00	0/1611	1.67	28/2195 (1.3%)
1	C	1.04	2/1611 (0.1%)	1.55	18/2195 (0.8%)
1	D	1.04	0/1611	1.68	26/2195 (1.2%)
1	E	1.05	0/1611	1.60	23/2195 (1.0%)
1	F	1.07	1/1611 (0.1%)	1.69	25/2195 (1.1%)
2	M	1.12	1/1895 (0.1%)	1.77	31/2580 (1.2%)
2	N	1.08	1/1895 (0.1%)	1.61	20/2580 (0.8%)
2	O	1.11	0/1895	1.64	30/2580 (1.2%)
2	P	1.12	2/1895 (0.1%)	1.75	36/2580 (1.4%)
2	Q	1.10	0/1895	1.67	27/2580 (1.0%)
2	R	1.11	0/1895	1.66	29/2580 (1.1%)
All	All	1.07	8/21036 (0.0%)	1.67	328/28650 (1.1%)

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	C	0	1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	94	ARG	CD-NE	-8.33	1.32	1.46
2	P	428	ARG	CD-NE	-6.71	1.35	1.46
1	C	66	SER	CA-CB	-6.19	1.43	1.52
2	N	438	SER	CB-OG	6.04	1.50	1.42
1	C	194	GLU	CD-OE2	-5.47	1.19	1.25
1	F	94	ARG	CD-NE	-5.10	1.37	1.46

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	440	ARG	CD-NE	-5.09	1.37	1.46
2	P	376	GLU	CD-OE1	-5.00	1.20	1.25

All (328) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	94	ARG	CD-NE-CZ	23.45	156.43	123.60
2	P	440	ARG	NE-CZ-NH2	-21.83	109.38	120.30
2	M	428	ARG	NE-CZ-NH1	19.34	129.97	120.30
2	M	440	ARG	NE-CZ-NH2	-18.06	111.27	120.30
1	D	94	ARG	NE-CZ-NH2	-16.78	111.91	120.30
1	F	38	ARG	NE-CZ-NH1	16.53	128.56	120.30
2	M	440	ARG	NE-CZ-NH1	16.33	128.47	120.30
2	P	428	ARG	NE-CZ-NH1	16.11	128.36	120.30
1	D	133	ARG	CD-NE-CZ	15.91	145.88	123.60
2	Q	440	ARG	NE-CZ-NH2	-15.80	112.40	120.30
2	Q	457	ARG	NE-CZ-NH1	14.96	127.78	120.30
2	N	440	ARG	NE-CZ-NH2	-14.86	112.87	120.30
1	B	184	ARG	NE-CZ-NH2	-14.86	112.87	120.30
1	E	38	ARG	NE-CZ-NH2	-14.49	113.05	120.30
2	Q	450	ARG	CD-NE-CZ	14.37	143.72	123.60
2	R	440	ARG	NE-CZ-NH2	-14.35	113.13	120.30
1	A	133	ARG	NE-CZ-NH1	14.11	127.36	120.30
2	R	428	ARG	NE-CZ-NH1	14.02	127.31	120.30
2	R	428	ARG	NE-CZ-NH2	-13.51	113.54	120.30
1	F	94	ARG	NE-CZ-NH1	13.23	126.92	120.30
2	P	440	ARG	NE-CZ-NH1	13.23	126.91	120.30
1	A	133	ARG	NE-CZ-NH2	-13.21	113.69	120.30
2	P	428	ARG	CG-CD-NE	12.74	138.56	111.80
2	O	428	ARG	NE-CZ-NH1	12.71	126.66	120.30
2	M	428	ARG	NE-CZ-NH2	-12.56	114.02	120.30
1	B	94	ARG	NE-CZ-NH1	12.24	126.42	120.30
2	P	307	ARG	NE-CZ-NH1	11.84	126.22	120.30
1	B	94	ARG	NE-CZ-NH2	-11.82	114.39	120.30
1	C	133	ARG	NE-CZ-NH1	11.58	126.09	120.30
1	A	94	ARG	CG-CD-NE	11.34	135.62	111.80
2	O	440	ARG	NE-CZ-NH2	-11.27	114.66	120.30
1	E	38	ARG	NE-CZ-NH1	11.26	125.93	120.30
1	D	133	ARG	NE-CZ-NH1	11.14	125.87	120.30
1	F	94	ARG	NE-CZ-NH2	-11.13	114.73	120.30
1	B	133	ARG	NE-CZ-NH2	-11.05	114.77	120.30
1	F	38	ARG	NE-CZ-NH2	-10.98	114.81	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	174	ARG	NE-CZ-NH1	10.97	125.78	120.30
1	D	94	ARG	NE-CZ-NH1	10.94	125.77	120.30
1	A	94	ARG	NE-CZ-NH2	-10.87	114.87	120.30
1	F	38	ARG	CD-NE-CZ	10.78	138.69	123.60
1	F	94	ARG	CD-NE-CZ	10.72	138.61	123.60
2	O	428	ARG	NE-CZ-NH2	-10.48	115.06	120.30
2	M	428	ARG	CD-NE-CZ	10.47	138.26	123.60
2	P	428	ARG	CD-NE-CZ	10.46	138.25	123.60
1	E	94	ARG	NE-CZ-NH1	10.41	125.50	120.30
2	O	428	ARG	CD-NE-CZ	10.10	137.74	123.60
1	F	133	ARG	NE-CZ-NH2	-10.05	115.28	120.30
2	Q	311	ARG	NE-CZ-NH1	10.04	125.32	120.30
2	O	333	ARG	NE-CZ-NH1	10.03	125.31	120.30
2	N	457	ARG	NE-CZ-NH2	-10.00	115.30	120.30
2	Q	457	ARG	NE-CZ-NH2	-9.98	115.31	120.30
1	B	38	ARG	NE-CZ-NH2	-9.92	115.34	120.30
2	Q	330	ARG	NE-CZ-NH2	-9.88	115.36	120.30
2	M	528	ARG	NE-CZ-NH2	-9.85	115.38	120.30
2	O	528	ARG	NE-CZ-NH2	-9.83	115.39	120.30
2	N	311	ARG	NE-CZ-NH2	-9.78	115.41	120.30
2	M	313	ARG	NE-CZ-NH1	9.77	125.19	120.30
2	Q	522	ARG	NE-CZ-NH1	-9.73	115.44	120.30
1	A	166	ARG	NE-CZ-NH1	9.45	125.03	120.30
1	D	166	ARG	NE-CZ-NH1	9.44	125.02	120.30
1	A	94	ARG	NE-CZ-NH1	9.42	125.01	120.30
1	D	133	ARG	NE-CZ-NH2	-9.31	115.64	120.30
1	C	133	ARG	CD-NE-CZ	9.30	136.63	123.60
2	P	450	ARG	CB-CG-CD	9.28	135.72	111.60
1	E	31	ARG	NE-CZ-NH1	9.23	124.92	120.30
1	F	133	ARG	NE-CZ-NH1	9.17	124.88	120.30
1	C	133	ARG	NE-CZ-NH2	-9.04	115.78	120.30
1	C	184	ARG	NE-CZ-NH1	9.04	124.82	120.30
2	P	524	ASP	CB-CG-OD1	9.02	126.42	118.30
1	A	38	ARG	NE-CZ-NH2	-9.02	115.79	120.30
1	A	184	ARG	NE-CZ-NH2	-9.02	115.79	120.30
2	R	522	ARG	NE-CZ-NH1	8.98	124.79	120.30
1	B	133	ARG	NE-CZ-NH1	8.97	124.79	120.30
2	N	528	ARG	NE-CZ-NH2	-8.97	115.82	120.30
2	R	457	ARG	NE-CZ-NH2	-8.94	115.83	120.30
1	B	188	ARG	NE-CZ-NH1	8.88	124.74	120.30
2	Q	311	ARG	NE-CZ-NH2	-8.84	115.88	120.30
1	C	166	ARG	NE-CZ-NH1	8.83	124.72	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	188	ARG	NE-CZ-NH1	8.75	124.68	120.30
2	O	407	ARG	NE-CZ-NH2	-8.73	115.94	120.30
2	O	333	ARG	NE-CZ-NH2	-8.71	115.94	120.30
2	O	330	ARG	NE-CZ-NH2	-8.70	115.95	120.30
2	O	432	ASP	CB-CG-OD2	-8.70	110.47	118.30
1	B	184	ARG	NE-CZ-NH1	8.68	124.64	120.30
1	D	65	ASP	CB-CG-OD1	8.62	126.06	118.30
2	R	522	ARG	CD-NE-CZ	8.61	135.66	123.60
1	A	38	ARG	NE-CZ-NH1	8.54	124.57	120.30
2	R	524	ASP	CB-CG-OD1	8.53	125.98	118.30
2	O	407	ARG	NE-CZ-NH1	8.52	124.56	120.30
2	M	407	ARG	NE-CZ-NH1	8.48	124.54	120.30
2	M	376	GLU	OE1-CD-OE2	8.42	133.40	123.30
2	Q	414	ARG	NE-CZ-NH1	8.37	124.48	120.30
1	D	184	ARG	NE-CZ-NH2	-8.35	116.13	120.30
1	B	167	ARG	NE-CZ-NH1	8.33	124.47	120.30
2	R	447	TYR	CB-CG-CD1	-8.31	116.02	121.00
1	B	167	ARG	NE-CZ-NH2	-8.27	116.17	120.30
2	R	407	ARG	NE-CZ-NH1	8.21	124.40	120.30
2	Q	524	ASP	CB-CG-OD2	-8.16	110.96	118.30
2	P	522	ARG	CD-NE-CZ	8.15	135.01	123.60
2	Q	450	ARG	NE-CZ-NH1	8.11	124.36	120.30
2	Q	383	ARG	NE-CZ-NH2	-8.09	116.26	120.30
2	P	313	ARG	NE-CZ-NH1	8.06	124.33	120.30
2	R	407	ARG	NE-CZ-NH2	-8.06	116.27	120.30
2	R	531	ARG	NE-CZ-NH2	-8.01	116.30	120.30
2	N	407	ARG	NE-CZ-NH1	7.83	124.22	120.30
2	Q	376	GLU	OE1-CD-OE2	7.78	132.64	123.30
2	O	517	ASP	CB-CG-OD1	7.76	125.28	118.30
1	F	133	ARG	CD-NE-CZ	7.68	134.35	123.60
2	M	524	ASP	CB-CG-OD2	-7.67	111.40	118.30
2	P	457	ARG	NE-CZ-NH2	-7.62	116.49	120.30
2	M	428	ARG	CG-CD-NE	7.54	127.63	111.80
1	B	94	ARG	CG-CD-NE	7.51	127.57	111.80
2	P	307	ARG	NE-CZ-NH2	-7.48	116.56	120.30
2	O	432	ASP	CB-CG-OD1	7.48	125.03	118.30
1	E	31	ARG	NE-CZ-NH2	-7.46	116.57	120.30
2	Q	428	ARG	NE-CZ-NH2	-7.44	116.58	120.30
1	A	74	ASP	CB-CG-OD1	7.42	124.98	118.30
2	M	509	ASP	CB-CG-OD1	7.31	124.88	118.30
2	P	432	ASP	CB-CG-OD2	-7.26	111.76	118.30
1	A	52	LEU	CB-CA-C	7.25	123.98	110.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	450	ARG	CD-NE-CZ	7.24	133.73	123.60
2	P	428	ARG	NE-CZ-NH2	-7.22	116.69	120.30
1	A	94	ARG	CB-CG-CD	7.15	130.20	111.60
2	P	432	ASP	CB-CG-OD1	7.15	124.74	118.30
1	C	36	TRP	CB-CA-C	7.12	124.64	110.40
1	B	94	ARG	CB-CG-CD	7.12	130.10	111.60
2	P	450	ARG	CG-CD-NE	7.09	126.68	111.80
1	E	186	ASP	CB-CG-OD1	7.09	124.68	118.30
1	B	188	ARG	NE-CZ-NH2	-7.08	116.76	120.30
1	F	142	ARG	NE-CZ-NH1	7.07	123.84	120.30
2	N	428	ARG	NE-CZ-NH2	-7.07	116.77	120.30
1	A	23	LEU	CB-CA-C	7.05	123.59	110.20
2	R	307	ARG	NE-CZ-NH1	7.02	123.81	120.30
2	M	531	ARG	NE-CZ-NH2	-7.00	116.80	120.30
2	P	536	GLU	CA-C-O	7.00	134.79	120.10
1	B	178	ASP	CB-CG-OD1	7.00	124.60	118.30
2	N	414	ARG	NE-CZ-NH1	6.98	123.79	120.30
1	A	32	ASP	CB-CG-OD1	6.98	124.58	118.30
1	B	36	TRP	CB-CA-C	6.98	124.35	110.40
2	Q	524	ASP	CB-CG-OD1	6.97	124.57	118.30
2	O	517	ASP	CB-CG-OD2	-6.93	112.07	118.30
2	O	383	ARG	NE-CZ-NH2	-6.92	116.84	120.30
1	D	174	ARG	NE-CZ-NH2	-6.91	116.84	120.30
2	R	376	GLU	OE1-CD-OE2	6.90	131.57	123.30
2	M	440	ARG	CD-NE-CZ	6.89	133.25	123.60
1	D	52	LEU	CB-CA-C	6.88	123.27	110.20
1	F	94	ARG	CG-CD-NE	6.85	126.18	111.80
2	P	383	ARG	NE-CZ-NH2	-6.83	116.88	120.30
1	A	36	TRP	CB-CA-C	6.83	124.06	110.40
2	R	524	ASP	CB-CG-OD2	-6.83	112.15	118.30
2	Q	330	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	D	186	ASP	CB-CG-OD1	6.81	124.43	118.30
2	P	524	ASP	CB-CG-OD2	-6.79	112.19	118.30
2	O	376	GLU	OE1-CD-OE2	6.74	131.39	123.30
2	M	457	ARG	NE-CZ-NH2	-6.74	116.93	120.30
1	F	36	TRP	CB-CA-C	6.74	123.87	110.40
1	F	158	LEU	CB-CA-C	6.71	122.95	110.20
2	N	409	ARG	NE-CZ-NH2	6.69	123.65	120.30
1	C	166	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	B	94	ARG	CD-NE-CZ	6.64	132.89	123.60
1	B	129	SER	N-CA-CB	6.62	120.43	110.50
2	R	509	ASP	CB-CG-OD1	6.57	124.22	118.30

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	330	ARG	NE-CZ-NH2	-6.56	117.02	120.30
2	R	428	ARG	CD-NE-CZ	6.56	132.79	123.60
2	N	409	ARG	NE-CZ-NH1	-6.55	117.02	120.30
1	F	23	LEU	CB-CA-C	6.53	122.61	110.20
1	F	57	ASP	CB-CG-OD2	-6.53	112.42	118.30
2	N	524	ASP	CB-CG-OD1	6.51	124.16	118.30
1	E	74	ASP	CB-CG-OD1	6.51	124.16	118.30
1	B	142	ARG	NE-CZ-NH2	-6.49	117.06	120.30
1	B	81	ASP	CB-CG-OD1	6.47	124.13	118.30
1	A	186	ASP	CB-CG-OD2	-6.46	112.48	118.30
1	A	184	ARG	NE-CZ-NH1	6.44	123.52	120.30
2	M	323	ASP	CB-CG-OD1	6.38	124.04	118.30
1	B	74	ASP	CB-CG-OD2	-6.32	112.61	118.30
1	A	52	LEU	CA-CB-CG	6.32	129.83	115.30
1	D	64	ARG	CD-NE-CZ	-6.32	114.76	123.60
1	D	188	ARG	CD-NE-CZ	-6.30	114.78	123.60
1	F	188	ARG	NE-CZ-NH2	-6.30	117.15	120.30
2	R	432	ASP	CB-CG-OD2	-6.29	112.63	118.30
2	R	437	TYR	CB-CG-CD1	-6.29	117.23	121.00
1	E	94	ARG	CG-CD-NE	6.29	125.00	111.80
1	F	166	ARG	NE-CZ-NH1	6.29	123.44	120.30
2	M	450	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	F	65	ASP	CB-CG-OD1	6.28	123.95	118.30
2	P	333	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	B	81	ASP	CB-CG-OD2	-6.26	112.66	118.30
1	D	94	ARG	CB-CG-CD	6.26	127.86	111.60
2	Q	450	ARG	NH1-CZ-NH2	-6.23	112.54	119.40
1	D	74	ASP	CB-CG-OD1	6.23	123.91	118.30
2	M	313	ARG	NE-CZ-NH2	-6.23	117.19	120.30
1	C	174	ARG	NE-CZ-NH1	6.22	123.41	120.30
2	N	304	ASP	CB-CG-OD1	6.21	123.89	118.30
1	A	64	ARG	NE-CZ-NH1	-6.20	117.20	120.30
2	O	313	ARG	NE-CZ-NH2	-6.20	117.20	120.30
2	N	528	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	C	158	LEU	CB-CA-C	6.18	121.95	110.20
2	P	333	ARG	CD-NE-CZ	6.17	132.24	123.60
2	R	440	ARG	NE-CZ-NH1	6.16	123.38	120.30
2	N	447	TYR	CB-CG-CD1	-6.14	117.32	121.00
1	C	52	LEU	CB-CA-C	6.14	121.86	110.20
2	N	432	ASP	CB-CG-OD1	6.13	123.81	118.30
1	D	43	ASP	CB-CG-OD2	-6.12	112.79	118.30
2	Q	499	GLU	CB-CG-CD	6.09	130.64	114.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	184	ARG	NE-CZ-NH1	6.07	123.34	120.30
2	N	452	GLY	N-CA-C	-6.07	97.93	113.10
2	R	376	GLU	CG-CD-OE2	-6.06	106.19	118.30
1	C	66	SER	N-CA-CB	6.06	119.58	110.50
1	A	100	ASP	CB-CG-OD2	6.04	123.74	118.30
1	D	162	GLU	CA-CB-CG	6.04	126.69	113.40
2	R	383	ARG	NE-CZ-NH2	-6.03	117.28	120.30
1	C	31	ARG	NE-CZ-NH2	-6.01	117.30	120.30
2	Q	372	LEU	CA-CB-CG	6.01	129.12	115.30
1	C	66	SER	CA-CB-OG	5.98	127.34	111.20
1	B	178	ASP	CB-CG-OD2	-5.98	112.92	118.30
1	A	75	ALA	CB-CA-C	5.97	119.05	110.10
2	O	353	HIS	CA-CB-CG	-5.97	103.46	113.60
1	A	141	THR	CA-CB-CG2	5.96	120.74	112.40
2	R	313	ARG	NE-CZ-NH1	5.93	123.26	120.30
2	M	383	ARG	NE-CZ-NH2	-5.92	117.34	120.30
2	P	509	ASP	CB-CG-OD1	5.88	123.59	118.30
1	E	133	ARG	NE-CZ-NH2	-5.88	117.36	120.30
2	Q	499	GLU	CG-CD-OE1	5.87	130.04	118.30
1	C	38	ARG	CD-NE-CZ	-5.84	115.42	123.60
2	M	432	ASP	CB-CG-OD2	-5.84	113.05	118.30
2	M	323	ASP	CB-CG-OD2	-5.83	113.06	118.30
2	O	447	TYR	CB-CG-CD2	-5.82	117.51	121.00
1	E	36	TRP	CB-CA-C	5.81	122.02	110.40
1	E	52	LEU	CB-CA-C	5.80	121.22	110.20
1	B	192	GLU	CA-CB-CG	5.80	126.15	113.40
1	D	94	ARG	CG-CD-NE	5.78	123.94	111.80
2	P	361	HIS	CA-CB-CG	-5.77	103.80	113.60
2	P	450	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	D	75	ALA	CB-CA-C	5.76	118.74	110.10
2	P	311	ARG	CG-CD-NE	-5.75	99.73	111.80
2	P	417	ALA	CB-CA-C	5.72	118.68	110.10
1	E	142	ARG	NE-CZ-NH2	-5.72	117.44	120.30
2	P	416	LEU	CA-CB-CG	5.70	128.41	115.30
2	P	428	ARG	CB-CG-CD	5.68	126.38	111.60
1	D	23	LEU	CB-CA-C	5.68	120.99	110.20
1	A	188	ARG	NE-CZ-NH2	-5.67	117.46	120.30
1	D	38	ARG	CD-NE-CZ	-5.67	115.66	123.60
1	C	188	ARG	NE-CZ-NH1	5.65	123.13	120.30
2	M	473	LYS	CA-CB-CG	5.65	125.83	113.40
1	D	78	GLU	OE1-CD-OE2	5.64	130.07	123.30
1	E	186	ASP	CB-CG-OD2	-5.64	113.22	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	398	GLU	OE1-CD-OE2	5.64	130.07	123.30
1	B	167	ARG	CD-NE-CZ	5.64	131.49	123.60
1	A	31	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	A	64	ARG	CD-NE-CZ	-5.61	115.75	123.60
1	D	64	ARG	NE-CZ-NH1	-5.61	117.50	120.30
1	F	52	LEU	CB-CA-C	5.60	120.84	110.20
2	Q	499	GLU	OE1-CD-OE2	-5.59	116.59	123.30
2	N	407	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	E	167	ARG	CD-NE-CZ	-5.57	115.80	123.60
2	P	478	LEU	CA-CB-CG	5.56	128.09	115.30
2	O	457	ARG	CA-CB-CG	5.56	125.63	113.40
1	A	174	ARG	NE-CZ-NH2	-5.55	117.52	120.30
1	F	94	ARG	CB-CG-CD	5.54	126.02	111.60
2	N	481	GLU	CA-CB-CG	5.54	125.58	113.40
1	E	142	ARG	NE-CZ-NH1	5.53	123.07	120.30
2	M	360	ASP	CB-CG-OD1	5.52	123.27	118.30
1	A	147	ASP	CB-CG-OD2	-5.50	113.35	118.30
1	F	158	LEU	CA-CB-CG	5.50	127.95	115.30
2	P	519	LEU	CB-CA-C	5.49	120.64	110.20
1	B	52	LEU	CA-CB-CG	5.49	127.93	115.30
1	E	100	ASP	CB-CG-OD1	-5.48	113.37	118.30
2	O	400	TRP	N-CA-CB	5.46	120.42	110.60
1	A	65	ASP	CB-CG-OD1	5.44	123.20	118.30
2	M	447	TYR	CB-CG-CD1	-5.44	117.73	121.00
2	O	522	ARG	NE-CZ-NH2	5.44	123.02	120.30
1	A	186	ASP	CB-CG-OD1	5.44	123.20	118.30
1	E	24	GLU	CB-CG-CD	5.44	128.88	114.20
1	E	74	ASP	CB-CG-OD2	-5.43	113.41	118.30
1	B	38	ARG	N-CA-CB	-5.42	100.84	110.60
2	O	440	ARG	NE-CZ-NH1	5.40	123.00	120.30
2	M	434	ASP	CB-CG-OD2	-5.39	113.45	118.30
2	N	417	ALA	CB-CA-C	5.38	118.17	110.10
2	M	507	LYS	CA-CB-CG	5.36	125.20	113.40
2	M	313	ARG	CB-CA-C	5.36	121.12	110.40
2	M	330	ARG	CD-NE-CZ	5.34	131.08	123.60
2	O	411	LYS	CB-CA-C	-5.34	99.72	110.40
2	R	361	HIS	CA-CB-CG	-5.34	104.53	113.60
1	D	166	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	B	13	ALA	CB-CA-C	5.32	118.07	110.10
2	N	428	ARG	NE-CZ-NH1	5.31	122.95	120.30
2	O	528	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	A	166	ARG	NE-CZ-NH2	-5.29	117.65	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	57	ASP	CB-CG-OD1	5.28	123.05	118.30
1	A	146	ASP	CB-CG-OD1	5.26	123.03	118.30
1	A	140	HIS	CB-CA-C	-5.26	99.88	110.40
1	C	19	ILE	CA-CB-CG2	5.24	121.38	110.90
1	E	158	LEU	CB-CA-C	5.24	120.16	110.20
2	M	531	ARG	NE-CZ-NH1	5.23	122.92	120.30
2	Q	450	ARG	NE-CZ-NH2	5.23	122.91	120.30
2	R	452	GLY	N-CA-C	-5.22	100.05	113.10
2	P	314	ASN	CB-CA-C	5.22	120.84	110.40
2	N	450	ARG	NE-CZ-NH1	5.21	122.90	120.30
2	R	386	ASP	CB-CA-C	5.20	120.81	110.40
2	O	499	GLU	CG-CD-OE1	5.20	128.69	118.30
2	Q	452	GLY	N-CA-C	-5.19	100.11	113.10
2	O	360	ASP	CB-CG-OD2	-5.19	113.63	118.30
2	P	481	GLU	CA-CB-CG	5.19	124.82	113.40
1	E	81	ASP	CB-CG-OD1	5.17	122.95	118.30
2	M	330	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	E	133	ARG	CD-NE-CZ	-5.16	116.38	123.60
2	R	411	LYS	CB-CA-C	-5.15	100.10	110.40
1	A	81	ASP	CB-CG-OD2	-5.14	113.67	118.30
1	B	162	GLU	CA-CB-CG	5.14	124.70	113.40
1	C	180	LYS	N-CA-CB	5.14	119.84	110.60
2	O	436	TYR	CB-CG-CD2	5.12	124.07	121.00
1	F	13	ALA	CB-CA-C	5.12	117.78	110.10
1	A	158	LEU	CB-CA-C	5.12	119.92	110.20
2	R	307	ARG	NE-CZ-NH2	-5.12	117.74	120.30
2	P	413	ASP	CB-CG-OD1	5.11	122.89	118.30
2	P	452	GLY	N-CA-C	-5.10	100.35	113.10
1	C	167	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	E	24	GLU	CA-CB-CG	5.09	124.60	113.40
2	Q	432	ASP	CB-CG-OD1	5.08	122.87	118.30
2	Q	432	ASP	CB-CG-OD2	-5.08	113.73	118.30
2	Q	361	HIS	CA-CB-CG	-5.07	104.98	113.60
1	E	81	ASP	CB-CG-OD2	-5.06	113.74	118.30
2	P	313	ARG	CD-NE-CZ	5.04	130.65	123.60
2	O	376	GLU	CG-CD-OE2	-5.03	108.24	118.30
2	Q	324	TYR	N-CA-C	-5.02	97.44	111.00
1	F	52	LEU	CA-CB-CG	5.02	126.85	115.30
2	O	531	ARG	NE-CZ-NH1	5.02	122.81	120.30
2	P	457	ARG	CD-NE-CZ	5.02	130.62	123.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	184	ARG	Sidechain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1571	0	1499	42	0
1	B	1571	0	1499	48	0
1	C	1571	0	1499	64	0
1	D	1571	0	1499	54	0
1	E	1571	0	1499	57	0
1	F	1571	0	1499	81	0
2	M	1840	0	1792	51	0
2	N	1840	0	1792	48	0
2	O	1840	0	1792	47	0
2	P	1840	0	1792	51	0
2	Q	1840	0	1792	62	0
2	R	1840	0	1792	72	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
3	O	1	0	0	0	0
3	P	1	0	0	0	0
3	Q	1	0	0	0	0
3	R	1	0	0	0	0
4	M	4	0	5	0	0
4	N	4	0	5	0	0
4	O	4	0	5	2	0
4	P	4	0	5	0	0
4	Q	4	0	5	3	0
4	R	4	0	5	2	0
5	M	22	0	7	0	0
5	N	22	0	7	0	0
5	O	22	0	7	2	0
5	P	22	0	7	0	0
5	Q	22	0	7	2	0
5	R	22	0	7	2	0
6	A	85	0	0	3	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	80	0	0	1	0
6	C	86	0	0	1	0
6	D	80	0	0	1	0
6	E	84	0	0	3	0
6	F	83	0	0	2	0
6	M	158	0	0	5	0
6	N	166	0	0	4	0
6	O	155	0	0	3	0
6	P	155	0	0	3	0
6	Q	159	0	0	7	0
6	R	161	0	0	4	0
All	All	22080	0	19818	600	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 (600) 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:D:64:ARG:NH1	1:D:100:ASP:O	1.88	1.06
1:F:64:ARG:NH1	1:F:100:ASP:O	1.87	1.04
1:E:165:GLN:NE2	1:E:165:GLN:H	1.59	0.99
1:B:165:GLN:NE2	1:B:165:GLN:H	1.59	0.99
1:C:64:ARG:NH1	1:C:100:ASP:O	1.98	0.97
1:F:163:GLN:HB3	1:F:165:GLN:NE2	1.82	0.95
1:F:163:GLN:HB3	1:F:165:GLN:HE22	1.31	0.95
1:E:64:ARG:NH1	1:E:100:ASP:O	2.01	0.93
1:B:163:GLN:HB3	1:B:165:GLN:NE2	1.83	0.92
2:R:364:LEU:HD22	2:R:440:ARG:HD3	1.52	0.92
2:M:390:LYS:HD2	6:M:640:HOH:O	1.70	0.90
1:F:168:GLU:HA	1:F:171:ILE:HD13	1.53	0.89
1:E:165:GLN:N	1:E:165:GLN:HE21	1.69	0.89
1:D:165:GLN:H	1:D:165:GLN:HE21	1.17	0.87
2:R:361:HIS:H	2:R:361:HIS:CD2	1.91	0.86
1:B:64:ARG:NH1	1:B:100:ASP:O	2.09	0.86
1:E:165:GLN:H	1:E:165:GLN:HE21	0.86	0.85
1:F:165:GLN:NE2	1:F:165:GLN:H	1.74	0.85
1:B:163:GLN:HB3	1:B:165:GLN:HE22	1.41	0.85
1:C:163:GLN:HB3	1:C:165:GLN:NE2	1.91	0.84
1:C:33:GLN:HG2	1:C:85:LEU:HD12	1.60	0.83
2:R:361:HIS:H	2:R:361:HIS:HD2	1.27	0.82

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:165:GLN:H	1:D:165:GLN:NE2	1.76	0.82
1:E:19:ILE:HG22	1:E:26:ALA:HB1	1.61	0.82
1:A:64:ARG:NH1	1:A:100:ASP:O	2.13	0.81
2:P:361:HIS:CD2	2:P:361:HIS:H	1.97	0.81
2:M:364:LEU:HD22	2:M:440:ARG:HD3	1.63	0.80
1:C:165:GLN:H	1:C:165:GLN:NE2	1.79	0.79
1:B:67:PHE:HZ	1:B:94:ARG:HD2	1.45	0.79
2:M:361:HIS:H	2:M:361:HIS:CD2	2.01	0.78
1:F:176:GLU:HG3	1:F:180:LYS:O	1.83	0.78
2:Q:438:SER:O	4:Q:601:BME:H22	1.83	0.78
2:M:356:PHE:HD1	2:M:428:ARG:HD3	1.49	0.77
1:A:67:PHE:HZ	1:A:94:ARG:HD2	1.48	0.77
2:Q:361:HIS:H	2:Q:361:HIS:CD2	2.02	0.77
2:P:361:HIS:HD2	2:P:361:HIS:H	1.31	0.75
2:O:364:LEU:HD22	2:O:440:ARG:HD3	1.69	0.75
1:F:165:GLN:CD	1:F:165:GLN:H	1.88	0.75
1:A:176:GLU:OE2	1:A:179:GLY:HA2	1.87	0.75
1:F:18:HIS:CE1	1:F:99:PHE:HE1	2.04	0.75
1:E:65:ASP:OD2	1:E:133:ARG:HD3	1.87	0.74
2:N:307:ARG:HG2	2:N:533:THR:HG22	1.68	0.74
2:R:473:LYS:HD2	2:R:474:LEU:N	2.02	0.74
2:Q:307:ARG:HG2	2:Q:533:THR:HG22	1.67	0.74
1:A:98:THR:HB	1:A:100:ASP:OD1	1.88	0.74
1:F:168:GLU:HA	1:F:171:ILE:CD1	2.17	0.74
2:O:361:HIS:CD2	2:O:361:HIS:H	2.04	0.74
1:F:78:GLU:HG2	2:R:301:PRO:CB	2.18	0.74
2:R:364:LEU:HD22	2:R:440:ARG:CD	2.18	0.74
1:B:70:VAL:HG21	1:B:106:LEU:HD21	1.68	0.73
1:D:24:GLU:OE1	1:D:25:ALA:N	2.21	0.73
2:Q:522:ARG:NH1	6:Q:689:HOH:O	2.22	0.73
1:B:61:HIS:ND1	1:C:163:GLN:HG3	2.04	0.73
1:C:24:GLU:OE1	1:C:25:ALA:N	2.21	0.73
1:C:41:LYS:NZ	1:C:86:GLU:O	2.22	0.73
1:C:16:TYR:O	1:C:19:ILE:HG23	1.89	0.73
1:E:132:ALA:HB3	1:E:135:ILE:HD12	1.71	0.72
2:M:326:THR:HG22	2:M:330:ARG:HD2	1.69	0.72
1:F:19:ILE:O	2:R:426:VAL:HG21	1.89	0.72
2:Q:361:HIS:H	2:Q:361:HIS:HD2	1.38	0.72
2:M:361:HIS:HD2	2:M:361:HIS:H	1.38	0.71
1:D:19:ILE:O	2:P:426:VAL:HG21	1.90	0.71
1:F:31:ARG:NH1	2:R:428:ARG:HG2	2.04	0.71

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:PHE:CZ	1:A:94:ARG:HD2	2.26	0.71
1:C:54:GLN:HG3	1:C:184:ARG:NH2	2.06	0.70
1:F:18:HIS:CE1	1:F:99:PHE:CE1	2.80	0.70
2:Q:416:LEU:C	2:Q:416:LEU:HD23	2.10	0.70
1:B:165:GLN:N	1:B:165:GLN:NE2	2.38	0.70
1:B:78:GLU:HG2	2:N:301:PRO:CB	2.22	0.69
1:D:67:PHE:HZ	1:D:94:ARG:HD2	1.57	0.69
2:P:405:GLY:HA3	6:P:682:HOH:O	1.92	0.69
2:R:383:ARG:HG3	2:R:436:TYR:CE1	2.26	0.69
1:A:78:GLU:HG2	2:M:301:PRO:HB3	1.74	0.68
1:A:78:GLU:HG2	2:M:301:PRO:CB	2.23	0.67
1:D:67:PHE:CZ	1:D:94:ARG:HD2	2.30	0.67
2:N:361:HIS:H	2:N:361:HIS:CD2	2.12	0.67
1:F:78:GLU:HG2	2:R:301:PRO:HG3	1.76	0.67
1:B:165:GLN:HE21	1:B:165:GLN:H	1.40	0.67
2:P:450:ARG:HD3	6:Q:622:HOH:O	1.93	0.67
2:M:304:ASP:HB2	2:M:343:ILE:HG13	1.76	0.67
1:B:24:GLU:OE1	1:B:25:ALA:N	2.29	0.66
1:B:67:PHE:CZ	1:B:94:ARG:HD2	2.30	0.66
1:A:176:GLU:HG3	1:A:180:LYS:O	1.96	0.66
1:F:98:THR:OG1	1:F:102:GLY:N	2.27	0.65
1:B:176:GLU:HG3	1:B:180:LYS:O	1.96	0.65
1:D:134:GLY:HA3	2:P:326:THR:HG22	1.79	0.65
2:M:356:PHE:CD1	2:M:428:ARG:HD3	2.31	0.65
2:M:364:LEU:HD22	2:M:440:ARG:CD	2.27	0.65
1:B:37:ASN:HB2	1:B:106:LEU:HD12	1.79	0.65
1:D:131:PHE:CE2	1:D:138:HIS:HB3	2.31	0.65
1:F:165:GLN:NE2	1:F:165:GLN:N	2.44	0.65
1:F:78:GLU:HG2	2:R:301:PRO:CG	2.27	0.65
2:P:442:ILE:HD12	2:P:442:ILE:O	1.97	0.65
1:E:19:ILE:HD11	2:Q:408:TYR:HD2	1.61	0.65
1:F:24:GLU:HG3	6:F:781:HOH:O	1.96	0.64
2:M:446:PRO:HD2	2:P:376:GLU:HG2	1.79	0.64
2:M:473:LYS:NZ	6:M:710:HOH:O	2.30	0.64
1:E:163:GLN:HB3	1:E:165:GLN:NE2	2.12	0.64
1:E:61:HIS:ND1	1:F:163:GLN:HG3	2.13	0.64
1:D:176:GLU:HG3	1:D:180:LYS:O	1.98	0.64
2:P:313:ARG:O	2:P:318:LYS:HE2	1.97	0.64
2:Q:361:HIS:CG	4:Q:601:BME:H21	2.32	0.64
2:Q:362:ASP:OD1	2:Q:440:ARG:HD3	1.98	0.64
1:A:176:GLU:HA	1:A:180:LYS:O	1.99	0.63

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:GLU:OE1	6:A:692:HOH:O	2.15	0.63
1:F:176:GLU:OE2	1:F:179:GLY:HA2	1.99	0.63
2:Q:363:LEU:HD23	2:Q:425:GLY:HA2	1.81	0.63
2:R:522:ARG:HH21	2:R:524:ASP:CG	2.02	0.63
2:O:361:HIS:HD2	2:O:361:HIS:H	1.46	0.63
1:D:35:ILE:HG21	1:D:92:PHE:HE1	1.64	0.63
1:E:67:PHE:HZ	1:E:94:ARG:HD2	1.64	0.63
2:P:359:HIS:O	2:P:366:ASN:HB3	1.98	0.63
1:B:131:PHE:CD2	1:B:138:HIS:HB3	2.35	0.62
1:E:176:GLU:OE2	1:E:179:GLY:HA2	1.99	0.62
1:A:24:GLU:CD	1:A:25:ALA:H	2.01	0.62
1:F:163:GLN:CB	1:F:165:GLN:HE22	2.10	0.62
1:B:78:GLU:HG2	2:N:301:PRO:CG	2.28	0.62
2:Q:447:TYR:HE1	5:Q:550:FHB:H5	1.64	0.62
1:B:180:LYS:HG2	1:B:181:THR:N	2.13	0.62
1:D:78:GLU:HG2	2:P:301:PRO:CG	2.30	0.62
2:M:360:ASP:OD2	2:M:428:ARG:HD2	2.00	0.62
2:N:522:ARG:NH1	6:N:774:HOH:O	2.15	0.61
1:B:165:GLN:N	1:B:165:GLN:HE21	1.97	0.61
2:M:522:ARG:NH1	6:M:665:HOH:O	2.26	0.61
1:E:98:THR:HB	1:E:100:ASP:OD1	2.00	0.61
1:F:78:GLU:CG	2:R:301:PRO:HG3	2.30	0.61
2:R:416:LEU:HD23	2:R:416:LEU:C	2.21	0.61
1:C:24:GLU:OE1	1:C:25:ALA:HB2	2.01	0.61
2:O:416:LEU:C	2:O:416:LEU:HD23	2.20	0.61
2:P:364:LEU:HD22	2:P:440:ARG:HD3	1.82	0.61
2:Q:473:LYS:NZ	6:Q:675:HOH:O	2.24	0.61
2:Q:361:HIS:ND1	4:Q:601:BME:H21	2.16	0.61
1:B:3:GLU:OE1	1:B:3:GLU:HA	2.00	0.60
1:E:131:PHE:CD2	1:E:138:HIS:HB3	2.36	0.60
1:C:143:LEU:HD23	1:C:143:LEU:C	2.22	0.60
1:F:134:GLY:HA3	2:R:326:THR:HG22	1.83	0.60
2:M:359:HIS:O	2:M:366:ASN:HB3	2.02	0.60
2:N:307:ARG:CG	2:N:533:THR:HG22	2.32	0.60
1:F:100:ASP:CG	1:F:101:ALA:H	2.05	0.60
2:N:359:HIS:O	2:N:366:ASN:HB3	2.01	0.60
2:R:408:TYR:HE2	2:R:447:TYR:CZ	2.19	0.60
2:R:522:ARG:NH2	2:R:524:ASP:OD1	2.35	0.60
1:C:168:GLU:HA	1:C:171:ILE:HD12	1.84	0.60
2:Q:390:LYS:HD2	6:Q:667:HOH:O	2.00	0.60
2:R:307:ARG:HG2	2:R:533:THR:HG22	1.83	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:390:LYS:HD2	6:N:749:HOH:O	2.00	0.60
2:O:361:HIS:CG	4:O:601:BME:H21	2.37	0.60
1:C:176:GLU:HG3	1:C:180:LYS:O	2.02	0.59
1:C:164:PRO:HA	1:C:167:ARG:HD2	1.83	0.59
1:B:163:GLN:CB	1:B:165:GLN:HE22	2.13	0.59
1:F:24:GLU:OE1	1:F:25:ALA:N	2.35	0.59
1:A:131:PHE:CD2	2:M:475:ILE:HD12	2.38	0.59
1:B:78:GLU:HG2	2:N:301:PRO:HB3	1.83	0.59
2:O:364:LEU:HD22	2:O:440:ARG:CD	2.32	0.59
2:N:376:GLU:O	2:N:442:ILE:HA	2.03	0.59
1:D:165:GLN:N	1:D:165:GLN:HE21	1.95	0.58
1:C:24:GLU:CD	1:C:25:ALA:H	2.07	0.58
1:B:39:LEU:HD11	1:B:93:GLY:HA3	1.86	0.58
1:A:163:GLN:HB3	1:A:165:GLN:HE21	1.68	0.58
1:C:165:GLN:H	1:C:165:GLN:HE21	1.51	0.58
1:C:19:ILE:O	2:O:426:VAL:HG21	2.04	0.58
1:D:78:GLU:HG2	2:P:301:PRO:CB	2.34	0.58
1:D:100:ASP:CG	1:D:101:ALA:H	2.06	0.58
1:E:168:GLU:HA	1:E:171:ILE:HD12	1.85	0.57
2:O:376:GLU:O	2:O:442:ILE:HA	2.04	0.57
1:C:51:LEU:HD12	1:C:106:LEU:HD23	1.86	0.57
2:M:400:TRP:HA	2:M:425:GLY:O	2.04	0.57
2:N:447:TYR:CE1	2:N:460:HIS:HE1	2.21	0.57
1:A:28:ASN:HB3	6:A:807:HOH:O	2.03	0.57
1:F:147:ASP:OD2	1:F:174:ARG:HD2	2.05	0.57
1:B:165:GLN:CD	1:B:165:GLN:H	2.04	0.57
1:D:176:GLU:OE2	1:D:179:GLY:HA2	2.04	0.57
2:Q:487:PRO:O	2:Q:493:LYS:HE2	2.05	0.57
2:P:447:TYR:CE2	2:P:460:HIS:HE1	2.23	0.57
1:A:144:TYR:CE1	1:A:158:LEU:HD13	2.40	0.56
1:A:24:GLU:OE1	1:A:25:ALA:HB2	2.05	0.56
2:N:478:LEU:HD12	2:N:523:PHE:CG	2.40	0.56
1:C:35:ILE:HG21	1:C:92:PHE:HE2	1.70	0.56
1:C:98:THR:O	1:C:102:GLY:HA2	2.05	0.56
1:D:98:THR:HB	1:D:100:ASP:OD1	2.06	0.56
1:F:67:PHE:HZ	1:F:94:ARG:HD2	1.70	0.56
2:P:363:LEU:HD23	2:P:425:GLY:HA2	1.88	0.56
2:N:326:THR:HG22	2:N:330:ARG:HD2	1.86	0.56
1:C:163:GLN:HB3	1:C:165:GLN:HE22	1.71	0.56
1:D:162:GLU:OE2	1:F:133:ARG:NH2	2.38	0.56
2:M:307:ARG:HG2	2:M:533:THR:HG22	1.86	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:131:PHE:O	1:F:132:ALA:HB2	2.05	0.56
2:Q:416:LEU:CD2	2:Q:416:LEU:C	2.73	0.56
1:E:66:SER:HB2	1:E:130:LEU:HD11	1.87	0.56
2:O:361:HIS:CD2	6:O:750:HOH:O	2.58	0.56
1:C:50:LEU:O	1:C:182:ALA:HA	2.05	0.55
2:M:448:PRO:CB	2:P:516:MET:HA	2.36	0.55
1:E:114:VAL:HG23	1:E:122:MET:HE3	1.87	0.55
1:E:4:LEU:HB3	2:Q:387:GLN:HB3	1.89	0.55
1:B:132:ALA:HB3	1:B:135:ILE:HD12	1.88	0.55
1:C:70:VAL:HG21	1:C:106:LEU:HD21	1.88	0.55
1:F:116:ASN:C	1:F:116:ASN:OD1	2.44	0.55
1:E:115:ASN:HA	1:E:121:PRO:HA	1.87	0.55
1:F:50:LEU:O	1:F:182:ALA:HA	2.06	0.55
1:C:54:GLN:HG3	1:C:184:ARG:HH22	1.71	0.55
2:O:478:LEU:C	2:O:478:LEU:HD23	2.27	0.55
1:E:78:GLU:HG2	2:Q:301:PRO:HB3	1.89	0.55
1:E:147:ASP:OD2	1:E:183:TYR:OH	2.19	0.55
1:F:150:GLN:O	1:F:153:ALA:HB3	2.06	0.55
2:R:405:GLY:HA3	6:R:787:HOH:O	2.06	0.55
1:B:98:THR:O	1:B:102:GLY:HA2	2.07	0.55
2:P:361:HIS:CD2	2:P:361:HIS:N	2.67	0.55
1:E:98:THR:O	1:E:102:GLY:HA2	2.06	0.54
1:F:35:ILE:HG22	1:F:94:ARG:HG3	1.89	0.54
1:C:41:LYS:HD2	1:C:88:ALA:HA	1.89	0.54
1:F:174:ARG:HE	1:F:181:THR:CG2	2.20	0.54
1:E:41:LYS:HD2	1:E:87:ASN:O	2.07	0.54
2:R:307:ARG:CG	2:R:533:THR:HG22	2.38	0.54
1:A:165:GLN:H	1:A:165:GLN:NE2	2.05	0.54
2:Q:447:TYR:CE1	5:Q:550:FHB:H5	2.40	0.54
1:A:163:GLN:HB3	1:A:165:GLN:NE2	2.23	0.54
1:F:31:ARG:N	1:F:34:GLU:OE2	2.26	0.54
2:P:364:LEU:HD11	2:P:442:ILE:HG23	1.90	0.54
1:A:131:PHE:CD2	1:A:138:HIS:HB3	2.43	0.54
1:C:24:GLU:HG3	6:C:781:HOH:O	2.08	0.54
2:Q:306:SER:CB	2:Q:530:GLN:HE21	2.20	0.54
1:B:19:ILE:O	2:N:426:VAL:HG21	2.07	0.54
1:E:32:ASP:HB2	6:E:810:HOH:O	2.08	0.53
1:A:69:GLU:OE1	2:M:473:LYS:HE2	2.07	0.53
2:N:307:ARG:NE	2:N:536:GLU:OE2	2.41	0.53
2:Q:376:GLU:O	2:Q:442:ILE:HA	2.08	0.53
1:C:176:GLU:OE2	1:C:179:GLY:HA2	2.07	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:38:ARG:HG3	1:D:107:HIS:HB2	1.91	0.53
2:O:356:PHE:HD1	2:O:428:ARG:HD2	1.73	0.53
2:R:383:ARG:HG3	2:R:436:TYR:CZ	2.44	0.53
1:F:180:LYS:HG2	1:F:181:THR:N	2.22	0.53
2:P:442:ILE:HD12	2:P:442:ILE:C	2.29	0.53
2:Q:400:TRP:HA	2:Q:425:GLY:O	2.09	0.53
1:A:39:LEU:HD11	1:A:93:GLY:HA3	1.90	0.53
1:E:176:GLU:HA	1:E:180:LYS:O	2.09	0.53
2:Q:364:LEU:HD11	2:Q:442:ILE:HG23	1.91	0.53
1:F:132:ALA:HB3	1:F:135:ILE:HD12	1.90	0.53
1:F:98:THR:O	1:F:102:GLY:HA2	2.08	0.53
1:A:41:LYS:HE3	1:A:87:ASN:O	2.09	0.53
1:E:131:PHE:O	1:E:132:ALA:HB2	2.08	0.53
2:O:486:ILE:N	2:O:487:PRO:HD2	2.24	0.53
1:B:131:PHE:CE2	1:B:138:HIS:HB3	2.44	0.52
1:A:100:ASP:CG	1:A:101:ALA:H	2.13	0.52
2:Q:408:TYR:HE1	2:Q:447:TYR:CE2	2.28	0.52
1:D:98:THR:OG1	1:D:102:GLY:N	2.37	0.52
1:B:65:ASP:OD2	1:B:133:ARG:HD3	2.10	0.52
1:F:98:THR:HG1	1:F:101:ALA:HB3	1.74	0.52
1:F:131:PHE:CD2	2:R:475:ILE:HD12	2.44	0.52
1:A:176:GLU:OE2	1:A:179:GLY:CA	2.56	0.52
2:M:360:ASP:HB3	2:M:428:ARG:HG3	1.92	0.52
2:R:447:TYR:CE2	5:R:550:FHB:H5	2.45	0.52
1:F:17:VAL:CG2	1:F:21:LEU:HD12	2.39	0.52
2:N:407:ARG:HD2	2:N:413:ASP:OD2	2.10	0.52
1:F:64:ARG:HD3	1:F:99:PHE:O	2.10	0.51
1:C:52:LEU:CD2	1:C:184:ARG:NH1	2.73	0.51
2:Q:399:MET:HA	2:Q:462:HIS:O	2.10	0.51
2:P:376:GLU:O	2:P:442:ILE:HA	2.10	0.51
2:N:447:TYR:HB2	2:N:448:PRO:HD2	1.93	0.51
2:O:360:ASP:HB3	2:O:428:ARG:HG3	1.92	0.51
1:F:19:ILE:O	2:R:426:VAL:CG2	2.56	0.51
1:E:50:LEU:O	1:E:182:ALA:HA	2.11	0.51
1:D:131:PHE:CD2	1:D:138:HIS:HB3	2.46	0.51
1:D:58:GLY:CA	1:D:190:GLN:HB3	2.40	0.51
2:M:405:GLY:HA3	6:M:643:HOH:O	2.10	0.51
1:B:24:GLU:CD	1:B:25:ALA:H	2.14	0.51
1:F:78:GLU:CD	2:R:301:PRO:HG3	2.31	0.51
1:F:84:ASN:O	1:F:87:ASN:HB2	2.10	0.51
1:E:24:GLU:O	1:E:27:GLY:N	2.42	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:376:GLU:HG2	2:P:446:PRO:HD2	1.92	0.51
2:M:448:PRO:HD3	2:M:456:TRP:CZ3	2.46	0.51
2:R:314:ASN:OD1	2:R:318:LYS:HE2	2.11	0.51
2:M:376:GLU:OE1	6:M:635:HOH:O	2.19	0.51
1:C:19:ILE:HG12	2:O:400:TRP:HB2	1.92	0.51
1:B:114:VAL:HG23	1:B:122:MET:HE2	1.92	0.50
1:D:19:ILE:HG13	2:P:400:TRP:HB2	1.91	0.50
1:D:65:ASP:OD2	1:D:133:ARG:HD3	2.11	0.50
1:E:24:GLU:OE1	1:E:25:ALA:N	2.36	0.50
2:M:465:ILE:N	2:M:465:ILE:HD12	2.25	0.50
2:R:486:ILE:HB	2:R:487:PRO:HD3	1.92	0.50
1:C:131:PHE:O	1:C:132:ALA:HB2	2.11	0.50
1:E:28:ASN:HB3	1:E:29:PRO:HD2	1.93	0.50
1:E:70:VAL:HG12	1:E:128:ILE:HG12	1.92	0.50
1:E:180:LYS:HG2	1:E:181:THR:N	2.27	0.50
1:F:49:ILE:CA	1:F:180:LYS:HE2	2.41	0.50
1:D:143:LEU:HD23	1:D:143:LEU:C	2.32	0.50
2:R:306:SER:CB	2:R:530:GLN:HE21	2.23	0.50
1:F:18:HIS:HE1	1:F:99:PHE:HE1	1.52	0.50
2:O:438:SER:O	4:O:601:BME:H22	2.12	0.50
2:M:377:ARG:CZ	2:P:416:LEU:HD21	2.42	0.50
1:E:39:LEU:HD11	1:E:93:GLY:HA3	1.94	0.50
1:F:180:LYS:CG	1:F:181:THR:N	2.75	0.50
1:E:69:GLU:OE1	2:Q:473:LYS:HE2	2.12	0.50
1:C:114:VAL:HG23	1:C:122:MET:CE	2.41	0.49
1:C:68:LEU:N	1:C:68:LEU:HD12	2.27	0.49
1:D:35:ILE:HG21	1:D:92:PHE:CE1	2.44	0.49
2:O:359:HIS:O	2:O:366:ASN:HB3	2.12	0.49
2:R:361:HIS:CG	4:R:601:BME:H21	2.47	0.49
1:A:131:PHE:CE2	1:A:138:HIS:HB3	2.47	0.49
1:A:165:GLN:H	1:A:165:GLN:CD	2.15	0.49
1:F:184:ARG:HG3	1:F:184:ARG:NH1	2.26	0.49
2:N:410:HIS:O	6:N:855:HOH:O	2.19	0.49
2:R:371:GLY:N	2:R:422:ASN:ND2	2.60	0.49
1:C:52:LEU:HD21	1:C:184:ARG:NH1	2.27	0.49
1:D:176:GLU:HG2	1:D:179:GLY:HA2	1.93	0.49
2:O:381:ALA:O	2:O:522:ARG:HA	2.13	0.49
2:Q:478:LEU:C	2:Q:478:LEU:HD23	2.32	0.49
2:R:392:VAL:HG12	2:R:395:THR:HB	1.94	0.49
1:D:50:LEU:O	1:D:182:ALA:HA	2.13	0.49
1:E:131:PHE:CE2	1:E:138:HIS:HB3	2.48	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:361:HIS:N	2:M:361:HIS:CD2	2.71	0.49
2:Q:460:HIS:HA	2:Q:478:LEU:O	2.11	0.49
1:D:24:GLU:O	1:D:27:GLY:N	2.42	0.49
1:A:4:LEU:HB3	2:M:387:GLN:HB3	1.94	0.49
2:N:415:TYR:CE1	2:N:416:LEU:HD22	2.47	0.49
2:Q:390:LYS:HD3	6:Q:745:HOH:O	2.12	0.49
1:B:50:LEU:HD12	1:B:51:LEU:N	2.27	0.49
1:C:163:GLN:HB3	1:C:165:GLN:HE21	1.75	0.49
2:N:534:HIS:CE1	2:P:512:ASN:O	2.66	0.49
1:C:100:ASP:OD1	1:C:100:ASP:N	2.45	0.49
1:D:84:ASN:OD1	1:D:86:GLU:HB2	2.12	0.49
1:F:67:PHE:CZ	1:F:94:ARG:HD2	2.47	0.49
2:N:362:ASP:OD2	2:N:440:ARG:NH1	2.46	0.49
2:Q:361:HIS:N	2:Q:361:HIS:CD2	2.73	0.49
1:C:165:GLN:N	1:C:165:GLN:HE21	2.11	0.49
2:M:448:PRO:HB2	2:P:516:MET:HA	1.94	0.49
1:D:133:ARG:HG3	2:P:326:THR:HG21	1.95	0.49
1:F:24:GLU:OE1	1:F:25:ALA:HB2	2.12	0.49
1:D:27:GLY:HA3	2:P:411:LYS:HE3	1.95	0.49
2:R:361:HIS:ND1	4:R:601:BME:H21	2.27	0.49
1:A:168:GLU:HA	1:A:171:ILE:HD12	1.94	0.48
1:A:24:GLU:OE1	1:A:25:ALA:N	2.45	0.48
1:C:52:LEU:HD22	1:C:52:LEU:C	2.33	0.48
1:F:125:HIS:HA	1:F:143:LEU:O	2.12	0.48
2:M:447:TYR:HB2	2:M:448:PRO:HD2	1.94	0.48
2:O:363:LEU:HD23	2:O:425:GLY:HA2	1.94	0.48
2:O:447:TYR:HB2	2:O:448:PRO:HD2	1.95	0.48
1:B:176:GLU:HG2	1:B:179:GLY:HA2	1.96	0.48
1:F:49:ILE:HA	1:F:180:LYS:HE2	1.94	0.48
1:A:19:ILE:HG21	2:M:410:HIS:HB2	1.95	0.48
2:N:447:TYR:CE1	2:N:460:HIS:CE1	3.01	0.48
2:Q:359:HIS:O	2:Q:366:ASN:HB3	2.13	0.48
1:E:176:GLU:HG3	1:E:180:LYS:O	2.13	0.48
2:M:392:VAL:HG12	2:M:395:THR:HB	1.95	0.48
2:Q:408:TYR:HE1	2:Q:447:TYR:CZ	2.31	0.48
2:R:400:TRP:HA	2:R:425:GLY:O	2.12	0.48
1:C:180:LYS:HG2	1:C:181:THR:N	2.28	0.48
1:F:171:ILE:N	1:F:171:ILE:HD12	2.29	0.48
2:R:363:LEU:HD12	2:R:363:LEU:N	2.29	0.48
2:R:531:ARG:NH1	2:R:532:LYS:O	2.44	0.48
1:C:35:ILE:HG21	1:C:92:PHE:CE2	2.47	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:78:GLU:HG2	2:O:301:PRO:CB	2.44	0.48
2:M:335:ALA:HB2	2:O:328:ILE:HD12	1.96	0.48
1:D:52:LEU:C	1:D:52:LEU:HD22	2.34	0.48
1:F:19:ILE:HG22	1:F:26:ALA:HB1	1.96	0.48
2:R:447:TYR:HE2	5:R:550:FHB:H5	1.78	0.48
1:E:24:GLU:CD	1:E:25:ALA:H	2.17	0.47
1:E:70:VAL:HG21	1:E:106:LEU:HD21	1.96	0.47
1:F:52:LEU:HD23	1:F:103:GLU:CD	2.34	0.47
2:Q:484:PRO:O	2:Q:487:PRO:HD2	2.14	0.47
1:C:67:PHE:C	1:C:68:LEU:HD12	2.34	0.47
1:E:37:ASN:HB2	1:E:106:LEU:HD12	1.95	0.47
1:E:20:GLY:HA2	2:Q:426:VAL:HG13	1.95	0.47
1:E:174:ARG:HE	1:E:181:THR:HG23	1.78	0.47
2:M:364:LEU:HB2	2:M:440:ARG:HD3	1.95	0.47
1:C:78:GLU:HG2	2:O:301:PRO:HG3	1.96	0.47
1:D:70:VAL:HG21	1:D:106:LEU:HD21	1.95	0.47
2:N:361:HIS:HD2	2:N:361:HIS:H	1.61	0.47
1:A:98:THR:OG1	1:A:102:GLY:N	2.44	0.47
1:D:36:TRP:CE3	1:D:36:TRP:HA	2.50	0.47
1:F:24:GLU:CD	1:F:25:ALA:H	2.18	0.47
1:F:50:LEU:HD12	1:F:51:LEU:N	2.30	0.47
2:P:416:LEU:HD23	2:P:416:LEU:C	2.35	0.47
2:Q:447:TYR:CE2	2:Q:460:HIS:HE1	2.32	0.47
1:D:78:GLU:HG2	2:P:301:PRO:HB3	1.95	0.47
1:F:116:ASN:OD1	1:F:118:ALA:N	2.48	0.47
2:P:408:TYR:HE2	2:P:447:TYR:CZ	2.33	0.47
2:Q:385:VAL:O	2:Q:526:VAL:HA	2.15	0.47
1:E:143:LEU:HD23	1:E:143:LEU:C	2.35	0.47
2:N:356:PHE:CD2	2:N:428:ARG:HD3	2.49	0.47
1:B:143:LEU:HD23	1:B:143:LEU:C	2.35	0.47
2:R:478:LEU:HD12	2:R:523:PHE:CD2	2.50	0.47
2:N:392:VAL:HG12	2:N:395:THR:HB	1.96	0.47
1:D:32:ASP:HB2	6:P:765:HOH:O	2.14	0.46
1:E:24:GLU:HG3	6:E:781:HOH:O	2.15	0.46
2:M:364:LEU:CD2	2:M:440:ARG:HD3	2.39	0.46
1:B:1:PRO:HB3	2:P:508:LEU:HB3	1.97	0.46
2:R:390:LYS:HE2	6:R:864:HOH:O	2.15	0.46
1:F:98:THR:OG1	1:F:101:ALA:HB3	2.14	0.46
2:M:385:VAL:O	2:M:526:VAL:HA	2.15	0.46
2:R:383:ARG:HA	2:R:435:GLY:O	2.16	0.46
2:Q:450:ARG:HD3	6:R:739:HOH:O	2.15	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:453:PRO:HB2	2:R:310:ILE:HD12	1.96	0.46
1:E:53:GLY:O	1:E:103:GLU:HG3	2.15	0.46
2:O:416:LEU:CD2	2:O:416:LEU:C	2.84	0.46
2:P:447:TYR:CE2	2:P:460:HIS:CE1	3.03	0.46
1:B:28:ASN:HB3	1:B:29:PRO:HD2	1.98	0.46
2:O:478:LEU:HD12	2:O:523:PHE:CD2	2.50	0.46
1:C:131:PHE:CD2	2:O:475:ILE:HD12	2.51	0.46
2:N:364:LEU:HD12	2:N:373:PRO:HG2	1.98	0.46
2:P:484:PRO:O	2:P:487:PRO:HD2	2.15	0.46
1:C:174:ARG:HE	1:C:181:THR:HG23	1.80	0.46
2:M:362:ASP:OD1	2:M:440:ARG:HD2	2.16	0.46
1:A:52:LEU:CD2	1:A:184:ARG:NH1	2.78	0.46
1:D:58:GLY:HA2	1:D:190:GLN:HB3	1.96	0.46
1:F:143:LEU:HD23	1:F:143:LEU:C	2.37	0.46
1:F:131:PHE:CE2	2:R:475:ILE:HD12	2.51	0.46
1:C:24:GLU:OE1	1:C:25:ALA:CB	2.65	0.45
2:O:447:TYR:HE1	5:O:550:FHB:H5	1.80	0.45
2:P:400:TRP:HA	2:P:425:GLY:O	2.15	0.45
1:C:28:ASN:HB3	1:C:29:PRO:HD2	1.98	0.45
1:E:199:ASP:CG	2:Q:313:ARG:HE	2.19	0.45
1:F:143:LEU:HD23	1:F:144:TYR:N	2.31	0.45
2:O:451:ASN:HB3	2:O:455:ASP:OD2	2.15	0.45
2:Q:390:LYS:HD3	6:Q:725:HOH:O	2.16	0.45
1:A:24:GLU:HG3	6:A:781:HOH:O	2.16	0.45
1:B:50:LEU:O	1:B:182:ALA:HA	2.15	0.45
1:E:35:ILE:HG21	1:E:92:PHE:HE2	1.81	0.45
2:N:399:MET:HA	2:N:462:HIS:O	2.15	0.45
2:P:360:ASP:OD2	2:P:428:ARG:HD2	2.16	0.45
2:Q:447:TYR:CE2	2:Q:460:HIS:CE1	3.05	0.45
2:R:411:LYS:O	2:R:414:ARG:NH2	2.49	0.45
2:M:478:LEU:C	2:M:478:LEU:HD23	2.37	0.45
2:R:302:ALA:HB1	2:R:347:THR:CG2	2.47	0.45
1:B:174:ARG:HE	1:B:181:THR:HG23	1.82	0.45
2:P:307:ARG:HD2	6:P:693:HOH:O	2.16	0.45
2:Q:489:CYS:HA	2:Q:490:PRO:HD3	1.71	0.45
1:F:155:CYS:O	1:F:159:ASN:ND2	2.46	0.45
2:P:448:PRO:HD3	2:P:456:TRP:CZ3	2.52	0.45
1:C:12:THR:HG21	2:O:324:TYR:OH	2.17	0.45
1:D:3:GLU:OE1	1:D:3:GLU:HA	2.17	0.45
1:F:146:ASP:HB3	1:F:171:ILE:CG2	2.47	0.45
2:R:416:LEU:HD23	2:R:417:ALA:N	2.32	0.45

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:489:CYS:HA	2:R:490:PRO:HD3	1.69	0.45
1:C:131:PHE:CD2	1:C:138:HIS:HB3	2.52	0.45
2:M:434:ASP:HB2	2:M:436:TYR:HD2	1.82	0.45
2:O:361:HIS:CD2	2:O:361:HIS:N	2.78	0.45
2:Q:448:PRO:HD3	2:Q:456:TRP:CZ3	2.52	0.45
1:F:3:GLU:OE1	1:F:3:GLU:HA	2.17	0.45
2:Q:431:THR:HG22	2:Q:437:TYR:HB3	1.99	0.45
2:N:408:TYR:HE1	2:N:447:TYR:CZ	2.35	0.44
2:N:497:ASN:HA	2:N:498:PRO:HD2	1.82	0.44
2:O:407:ARG:HD3	2:O:417:ALA:O	2.17	0.44
2:P:489:CYS:HA	2:P:490:PRO:HD3	1.80	0.44
2:R:408:TYR:HE2	2:R:447:TYR:CE1	2.35	0.44
2:Q:385:VAL:HA	2:Q:390:LYS:O	2.17	0.44
2:R:383:ARG:HB2	2:R:522:ARG:NH2	2.32	0.44
1:F:122:MET:HG2	1:F:156:PRO:HG2	1.99	0.44
2:M:512:ASN:O	2:Q:534:HIS:HE1	2.00	0.44
2:N:534:HIS:HE1	2:P:512:ASN:O	2.01	0.44
1:C:78:GLU:CG	2:O:301:PRO:HG3	2.48	0.44
1:D:147:ASP:OD2	1:D:183:TYR:OH	2.34	0.44
1:E:35:ILE:HG21	1:E:92:PHE:CE2	2.53	0.44
1:F:115:ASN:HA	1:F:121:PRO:HA	1.99	0.44
2:N:400:TRP:HA	2:N:425:GLY:O	2.17	0.44
2:O:522:ARG:NH1	6:O:716:HOH:O	2.24	0.44
2:Q:390:LYS:HG2	2:Q:391:PRO:O	2.18	0.44
1:A:35:ILE:HG21	1:A:92:PHE:HE1	1.82	0.44
2:Q:383:ARG:HA	2:Q:435:GLY:O	2.18	0.44
1:D:33:GLN:HG2	1:D:85:LEU:HD12	2.00	0.44
2:O:411:LYS:O	2:O:414:ARG:NH2	2.51	0.44
2:O:420:ASP:HA	2:O:421:PRO:HD2	1.79	0.44
1:C:123:ALA:HB3	1:C:144:TYR:CE2	2.53	0.44
1:D:168:GLU:HA	1:D:171:ILE:HD12	2.00	0.44
1:D:38:ARG:HH11	1:D:38:ARG:HD2	1.62	0.44
1:A:51:LEU:HD11	1:A:126:ILE:CD1	2.48	0.43
2:O:405:GLY:HA3	6:O:682:HOH:O	2.18	0.43
6:E:697:HOH:O	2:Q:426:VAL:HG21	2.17	0.43
2:Q:517:ASP:C	2:Q:517:ASP:OD1	2.54	0.43
2:R:447:TYR:CE1	2:R:460:HIS:HE1	2.36	0.43
1:A:50:LEU:O	1:A:182:ALA:HA	2.18	0.43
1:B:176:GLU:HG3	1:B:180:LYS:C	2.39	0.43
2:M:512:ASN:O	2:Q:534:HIS:CE1	2.71	0.43
2:R:360:ASP:OD2	2:R:428:ARG:HD2	2.18	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:94:ARG:NH2	2:R:398:GLU:OE2	2.39	0.43
1:C:19:ILE:HG21	1:C:19:ILE:HD13	1.60	0.43
1:F:47:GLU:O	1:F:49:ILE:HG23	2.19	0.43
1:D:163:GLN:HG3	1:F:61:HIS:ND1	2.33	0.43
2:R:307:ARG:NE	2:R:536:GLU:OE2	2.51	0.43
1:B:35:ILE:HG21	1:B:92:PHE:HE2	1.83	0.43
2:M:377:ARG:NE	2:P:416:LEU:HD21	2.33	0.43
2:N:447:TYR:HE1	2:N:460:HIS:CE1	2.36	0.43
2:N:493:LYS:HB2	2:N:493:LYS:HE3	1.74	0.43
1:C:64:ARG:HD3	1:C:99:PHE:O	2.18	0.43
1:C:73:ALA:HB1	1:C:78:GLU:N	2.34	0.43
1:E:58:GLY:HA2	1:E:190:GLN:HB3	2.01	0.43
2:R:372:LEU:HA	2:R:373:PRO:HD3	1.90	0.43
2:R:385:VAL:O	2:R:526:VAL:HA	2.18	0.43
1:B:24:GLU:O	1:B:27:GLY:N	2.45	0.43
1:F:98:THR:HB	1:F:100:ASP:OD1	2.18	0.43
2:P:468:PRO:HD2	2:P:472:THR:HG21	2.01	0.43
2:R:473:LYS:HD2	2:R:474:LEU:H	1.78	0.43
1:C:158:LEU:HA	1:C:158:LEU:HD12	1.91	0.43
1:C:165:GLN:H	1:C:165:GLN:CD	2.16	0.43
1:D:52:LEU:HD21	1:D:184:ARG:NH1	2.34	0.43
2:P:497:ASN:OD1	2:P:499:GLU:HB2	2.18	0.43
2:Q:408:TYR:CE1	2:Q:447:TYR:CE2	3.06	0.43
2:Q:453:PRO:HG2	2:R:310:ILE:HG23	2.00	0.43
1:F:31:ARG:HH11	2:R:428:ARG:HG2	1.81	0.43
1:C:114:VAL:HG23	1:C:122:MET:HE3	2.00	0.43
1:C:41:LYS:NZ	1:C:86:GLU:C	2.72	0.43
2:N:373:PRO:HB3	2:N:423:PHE:HB2	2.00	0.43
2:R:437:TYR:C	2:R:437:TYR:CD1	2.92	0.43
2:R:304:ASP:HA	6:R:876:HOH:O	2.18	0.43
2:R:361:HIS:N	2:R:361:HIS:CD2	2.64	0.43
1:B:131:PHE:CD2	2:N:475:ILE:HD12	2.54	0.43
1:D:98:THR:O	1:D:102:GLY:HA2	2.19	0.43
1:E:133:ARG:HH11	1:E:133:ARG:HD3	1.63	0.43
1:E:15:PRO:HB3	1:E:133:ARG:HD2	2.01	0.43
2:N:405:GLY:HA3	6:N:752:HOH:O	2.19	0.43
2:P:318:LYS:HD3	2:P:318:LYS:HA	1.74	0.43
2:Q:486:ILE:HB	2:Q:487:PRO:HD3	2.01	0.43
2:R:395:THR:O	2:R:430:LEU:HA	2.19	0.43
1:A:51:LEU:HD12	1:A:106:LEU:HD23	2.01	0.42
1:B:38:ARG:HA	1:B:107:HIS:HB2	2.01	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:VAL:HA	1:C:121:PRO:HD3	1.75	0.42
1:D:78:GLU:HG2	2:P:301:PRO:HG2	2.01	0.42
1:F:77:GLY:O	1:F:114:VAL:HG12	2.19	0.42
2:N:356:PHE:CE2	2:N:428:ARG:HD3	2.54	0.42
2:P:341:GLN:HB3	2:P:346:THR:CG2	2.48	0.42
1:E:131:PHE:CD2	2:Q:475:ILE:HD12	2.54	0.42
2:P:381:ALA:O	2:P:522:ARG:HA	2.19	0.42
2:R:386:ASP:HA	2:R:527:LEU:O	2.19	0.42
2:O:447:TYR:CE1	5:O:550:FHB:H5	2.55	0.42
1:C:11:GLN:HB2	2:O:477:GLN:HG3	2.00	0.42
2:R:416:LEU:CD2	2:R:416:LEU:C	2.88	0.42
1:A:54:GLN:HG2	1:A:102:GLY:O	2.18	0.42
1:D:116:ASN:OD1	1:D:116:ASN:C	2.57	0.42
1:F:176:GLU:OE2	1:F:179:GLY:CA	2.67	0.42
2:Q:405:GLY:HA3	6:Q:670:HOH:O	2.18	0.42
2:Q:441:THR:OG1	2:Q:442:ILE:N	2.52	0.42
1:B:19:ILE:O	2:N:426:VAL:CG2	2.67	0.42
1:C:78:GLU:HG2	2:O:301:PRO:HB3	2.00	0.42
1:F:134:GLY:HA3	2:R:326:THR:CG2	2.49	0.42
1:A:19:ILE:CG2	2:M:410:HIS:HB2	2.50	0.42
2:N:325:LYS:HG2	2:O:335:ALA:HB1	2.01	0.42
2:Q:497:ASN:HA	2:Q:498:PRO:HD2	1.78	0.42
2:N:383:ARG:NE	2:N:434:ASP:O	2.48	0.42
2:M:515:PRO:HB3	2:P:453:PRO:O	2.20	0.42
2:R:390:LYS:HA	2:R:391:PRO:HD3	1.90	0.42
1:D:24:GLU:HG3	6:D:781:HOH:O	2.19	0.42
1:F:100:ASP:CG	1:F:101:ALA:N	2.72	0.42
2:N:383:ARG:HG3	2:N:436:TYR:CE1	2.54	0.42
2:N:383:ARG:HA	2:N:435:GLY:O	2.20	0.42
1:B:62:LEU:HD12	1:B:64:ARG:NH2	2.35	0.41
2:R:497:ASN:HA	2:R:498:PRO:HD3	1.87	0.41
1:D:176:GLU:HG2	1:D:179:GLY:CA	2.50	0.41
1:D:51:LEU:HB2	1:D:106:LEU:HB3	2.03	0.41
2:N:306:SER:O	2:N:307:ARG:NH1	2.53	0.41
2:R:447:TYR:HB2	2:R:448:PRO:HD2	2.00	0.41
1:B:131:PHE:O	1:B:132:ALA:HB2	2.21	0.41
1:B:84:ASN:OD1	1:B:86:GLU:HB2	2.21	0.41
1:C:98:THR:OG1	1:C:101:ALA:HB3	2.20	0.41
2:N:416:LEU:C	2:N:416:LEU:HD23	2.41	0.41
2:R:321:THR:HG21	2:R:494:SER:HB2	2.02	0.41
2:O:519:LEU:HD23	2:O:519:LEU:HA	1.85	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:LEU:HD12	1:B:158:LEU:HA	1.88	0.41
1:E:24:GLU:OE1	1:E:25:ALA:CB	2.68	0.41
1:E:72:GLN:HB3	1:E:126:ILE:HG12	2.01	0.41
2:M:449:TRP:CZ3	2:M:451:ASN:HB2	2.55	0.41
1:A:180:LYS:CG	1:A:181:THR:N	2.84	0.41
1:C:140:HIS:O	1:C:197:PHE:HA	2.21	0.41
2:R:478:LEU:HD23	2:R:478:LEU:C	2.41	0.41
1:C:38:ARG:HG3	1:C:107:HIS:HB2	2.02	0.41
2:M:383:ARG:NE	2:M:434:ASP:O	2.47	0.41
2:M:364:LEU:HD11	2:M:442:ILE:HG23	2.02	0.41
2:P:447:TYR:CZ	2:P:460:HIS:HE1	2.39	0.41
1:E:146:ASP:HB3	1:E:171:ILE:HG22	2.03	0.41
1:F:12:THR:HA	1:F:135:ILE:O	2.21	0.41
1:F:15:PRO:HG2	1:F:16:TYR:CD2	2.56	0.41
2:N:363:LEU:HD11	2:N:427:GLY:HA3	2.02	0.41
2:O:493:LYS:HE3	2:O:493:LYS:HB2	1.90	0.41
1:E:19:ILE:HG21	2:Q:410:HIS:HB2	2.02	0.41
2:Q:315:TRP:CZ2	2:Q:500:ALA:HA	2.55	0.41
1:D:4:LEU:HB3	2:P:387:GLN:HB3	2.02	0.41
2:M:376:GLU:O	2:M:442:ILE:HA	2.21	0.41
2:N:489:CYS:HA	2:N:490:PRO:HD3	1.75	0.41
2:O:408:TYR:HE1	2:O:447:TYR:CZ	2.39	0.41
2:O:483:ASP:HA	2:O:484:PRO:HD2	1.94	0.41
1:B:24:GLU:HG3	6:B:781:HOH:O	2.20	0.40
2:N:447:TYR:HA	2:N:448:PRO:HD3	1.95	0.40
2:O:356:PHE:HD1	2:O:428:ARG:CD	2.33	0.40
1:A:143:LEU:HD23	1:A:143:LEU:C	2.41	0.40
2:N:390:LYS:HA	2:N:391:PRO:HD3	1.80	0.40
2:O:497:ASN:HA	2:O:498:PRO:HD2	1.81	0.40
2:R:420:ASP:HA	2:R:421:PRO:HD2	1.77	0.40
1:A:68:LEU:HD12	1:A:68:LEU:N	2.37	0.40
1:E:19:ILE:HG23	2:Q:410:HIS:HD2	1.86	0.40
2:M:489:CYS:HA	2:M:490:PRO:HD3	1.74	0.40
1:C:19:ILE:O	2:O:426:VAL:CG2	2.70	0.40
1:E:52:LEU:C	1:E:52:LEU:HD22	2.41	0.40
1:F:19:ILE:HG21	1:F:19:ILE:HD13	1.71	0.40
2:P:308:PHE:HA	2:P:529:GLY:O	2.22	0.40
2:R:331:SER:HA	2:R:332:PRO:HD3	1.91	0.40
2:R:486:ILE:N	2:R:487:PRO:CD	2.85	0.40
1:D:19:ILE:HG22	1:D:26:ALA:HB1	2.03	0.40
1:F:113:VAL:HA	6:F:680:HOH:O	2.22	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:478:LEU:HD12	2:O:523:PHE:CG	2.57	0.40
1:D:78:GLU:CG	2:P:301:PRO:HG2	2.52	0.40
2:Q:363:LEU:HD23	2:Q:425:GLY:CA	2.48	0.40
2:R:399:MET:HA	2:R:462:HIS:O	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	198/200 (99%)	192 (97%)	6 (3%)	0	100	100
1	B	198/200 (99%)	192 (97%)	6 (3%)	0	100	100
1	C	198/200 (99%)	193 (98%)	5 (2%)	0	100	100
1	D	198/200 (99%)	189 (96%)	9 (4%)	0	100	100
1	E	198/200 (99%)	188 (95%)	10 (5%)	0	100	100
1	F	198/200 (99%)	185 (93%)	13 (7%)	0	100	100
2	M	229/238 (96%)	219 (96%)	10 (4%)	0	100	100
2	N	229/238 (96%)	222 (97%)	7 (3%)	0	100	100
2	O	229/238 (96%)	221 (96%)	8 (4%)	0	100	100
2	P	229/238 (96%)	220 (96%)	9 (4%)	0	100	100
2	Q	229/238 (96%)	219 (96%)	10 (4%)	0	100	100
2	R	229/238 (96%)	219 (96%)	10 (4%)	0	100	100
All	All	2562/2628 (98%)	2459 (96%)	103 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	162/163 (99%)	154 (95%)	8 (5%)	25	21
1	B	162/163 (99%)	151 (93%)	11 (7%)	16	10
1	C	162/163 (99%)	156 (96%)	6 (4%)	34	32
1	D	162/163 (99%)	157 (97%)	5 (3%)	40	39
1	E	162/163 (99%)	155 (96%)	7 (4%)	29	27
1	F	162/163 (99%)	157 (97%)	5 (3%)	40	39
2	M	196/202 (97%)	186 (95%)	10 (5%)	24	20
2	N	196/202 (97%)	188 (96%)	8 (4%)	30	29
2	O	196/202 (97%)	186 (95%)	10 (5%)	24	20
2	P	196/202 (97%)	190 (97%)	6 (3%)	40	39
2	Q	196/202 (97%)	189 (96%)	7 (4%)	35	33
2	R	196/202 (97%)	186 (95%)	10 (5%)	24	20
All	All	2148/2190 (98%)	2055 (96%)	93 (4%)	29	27

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	19	ILE
1	A	24	GLU
1	A	38	ARG
1	A	52	LEU
1	A	114	VAL
1	A	133	ARG
1	A	165	GLN
2	M	364	LEU
2	M	372	LEU
2	M	395	THR
2	M	416	LEU
2	M	433	SER
2	M	440	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	M	446	PRO
2	M	450	ARG
2	M	473	LYS
2	M	534	HIS
1	B	4	LEU
1	B	19	ILE
1	B	24	GLU
1	B	32	ASP
1	B	38	ARG
1	B	52	LEU
1	B	133	ARG
1	B	158	LEU
1	B	165	GLN
1	B	176	GLU
1	B	184	ARG
2	N	364	LEU
2	N	372	LEU
2	N	395	THR
2	N	399	MET
2	N	416	LEU
2	N	428	ARG
2	N	450	ARG
2	N	534	HIS
1	C	4	LEU
1	C	19	ILE
1	C	24	GLU
1	C	52	LEU
1	C	100	ASP
1	C	165	GLN
2	O	326	THR
2	O	372	LEU
2	O	393	PRO
2	O	395	THR
2	O	399	MET
2	O	416	LEU
2	O	428	ARG
2	O	450	ARG
2	O	478	LEU
2	O	534	HIS
1	D	24	GLU
1	D	43	ASP
1	D	52	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	164	PRO
1	D	165	GLN
2	P	395	THR
2	P	399	MET
2	P	416	LEU
2	P	440	ARG
2	P	478	LEU
2	P	534	HIS
1	E	4	LEU
1	E	19	ILE
1	E	24	GLU
1	E	38	ARG
1	E	52	LEU
1	E	165	GLN
1	E	184	ARG
2	Q	372	LEU
2	Q	395	THR
2	Q	399	MET
2	Q	416	LEU
2	Q	428	ARG
2	Q	450	ARG
2	Q	534	HIS
1	F	4	LEU
1	F	19	ILE
1	F	24	GLU
1	F	52	LEU
1	F	165	GLN
2	R	372	LEU
2	R	383	ARG
2	R	395	THR
2	R	399	MET
2	R	416	LEU
2	R	428	ARG
2	R	440	ARG
2	R	450	ARG
2	R	473	LYS
2	R	534	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	163	GLN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	165	GLN
2	M	361	HIS
2	M	412	ASN
1	B	165	GLN
2	N	361	HIS
2	N	412	ASN
1	C	165	GLN
2	O	361	HIS
2	O	412	ASN
1	D	165	GLN
2	P	361	HIS
2	P	412	ASN
1	E	165	GLN
2	Q	361	HIS
2	Q	530	GLN
1	F	150	GLN
1	F	165	GLN
2	R	361	HIS
2	R	412	ASN
2	R	422	ASN
2	R	530	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](#)

Of 24 ligands modelled in this entry, 6 are monoatomic - leaving 18 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
5	FHB	R	551	-	9,11,11	1.83	1 (11%)	10,15,15	0.80	0
4	BME	R	601	2	3,3,3	0.61	0	1,2,2	1.15	0
5	FHB	M	550	3	9,11,11	1.82	2 (22%)	10,15,15	1.02	0
5	FHB	O	551	-	9,11,11	1.86	1 (11%)	10,15,15	1.04	0
5	FHB	O	550	3	9,11,11	1.67	2 (22%)	10,15,15	0.77	0
5	FHB	P	550	3	9,11,11	1.53	1 (11%)	10,15,15	0.86	0
5	FHB	R	550	3,2	9,11,11	1.16	1 (11%)	10,15,15	0.74	0
5	FHB	M	551	-	9,11,11	1.40	1 (11%)	10,15,15	0.63	0
4	BME	O	601	2	3,3,3	0.40	0	1,2,2	0.48	0
5	FHB	N	551	-	9,11,11	1.95	1 (11%)	10,15,15	0.78	0
4	BME	Q	601	2	3,3,3	0.60	0	1,2,2	0.81	0
5	FHB	N	550	3	9,11,11	2.15	1 (11%)	10,15,15	0.89	0
5	FHB	P	551	-	9,11,11	1.69	2 (22%)	10,15,15	1.06	0
5	FHB	Q	550	3	9,11,11	2.14	2 (22%)	10,15,15	1.31	1 (10%)
4	BME	M	601	2	3,3,3	0.18	0	1,2,2	0.13	0
4	BME	N	601	2	3,3,3	0.25	0	1,2,2	0.12	0
5	FHB	Q	551	-	9,11,11	1.78	1 (11%)	10,15,15	1.01	0
4	BME	P	601	2	3,3,3	0.30	0	1,2,2	0.04	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	FHB	R	551	-	-	0/0/4/4	0/1/1/1
4	BME	R	601	2	-	0/1/1/1	-
5	FHB	M	550	3	-	0/0/4/4	0/1/1/1
5	FHB	O	551	-	-	0/0/4/4	0/1/1/1
5	FHB	O	550	3	-	0/0/4/4	0/1/1/1
5	FHB	P	550	3	-	0/0/4/4	0/1/1/1
5	FHB	R	550	3,2	-	0/0/4/4	0/1/1/1
5	FHB	M	551	-	-	0/0/4/4	0/1/1/1
4	BME	O	601	2	-	0/1/1/1	-
5	FHB	N	551	-	-	0/0/4/4	0/1/1/1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BME	Q	601	2	-	0/1/1/1	-
5	FHB	N	550	3	-	0/0/4/4	0/1/1/1
5	FHB	P	551	-	-	0/0/4/4	0/1/1/1
5	FHB	Q	550	3	-	0/0/4/4	0/1/1/1
4	BME	M	601	2	-	1/1/1/1	-
4	BME	N	601	2	-	0/1/1/1	-
5	FHB	Q	551	-	-	0/0/4/4	0/1/1/1
4	BME	P	601	2	-	0/1/1/1	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	N	550	FHB	C1-C7	5.89	1.53	1.47
5	Q	550	FHB	C1-C7	5.58	1.52	1.47
5	N	551	FHB	C1-C7	5.41	1.52	1.47
5	O	551	FHB	C1-C7	4.87	1.52	1.47
5	R	551	FHB	C1-C7	4.82	1.52	1.47
5	M	550	FHB	C1-C7	4.60	1.51	1.47
5	Q	551	FHB	C1-C7	4.53	1.51	1.47
5	P	551	FHB	C1-C7	3.82	1.51	1.47
5	O	550	FHB	C1-C7	3.68	1.51	1.47
5	P	550	FHB	C1-C7	3.47	1.50	1.47
5	M	551	FHB	C1-C7	3.04	1.50	1.47
5	R	550	FHB	C1-C7	2.73	1.50	1.47
5	O	550	FHB	C4-C3	2.73	1.41	1.39
5	Q	550	FHB	C2-C1	2.35	1.43	1.39
5	P	551	FHB	C4-C3	2.19	1.41	1.39
5	M	550	FHB	C4-C3	2.01	1.40	1.39

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Q	550	FHB	C2-C1-C7	-2.59	116.94	120.36

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	M	601	BME	O1-C1-C2-S2

There are no ring outliers.

6 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	R	601	BME	2	0
5	O	550	FHB	2	0
5	R	550	FHB	2	0
4	O	601	BME	2	0
4	Q	601	BME	3	0
5	Q	550	FHB	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.