



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 18, 2023 – 02:47 PM EDT

PDB ID : 3PCE
Title : STRUCTURE OF PROTOCATECHUATE 3,4-DIOXYGENASE COM-
PLEXED WITH 3-HYDROXYPHENYLACETATE
Authors : Elango, N.; Orville, A.M.; Lipscomb, J.D.; Ohlendorf, D.H.
Deposited on : 1997-04-29
Resolution : 2.06 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

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)
Xtrriage (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) : 2.35.1

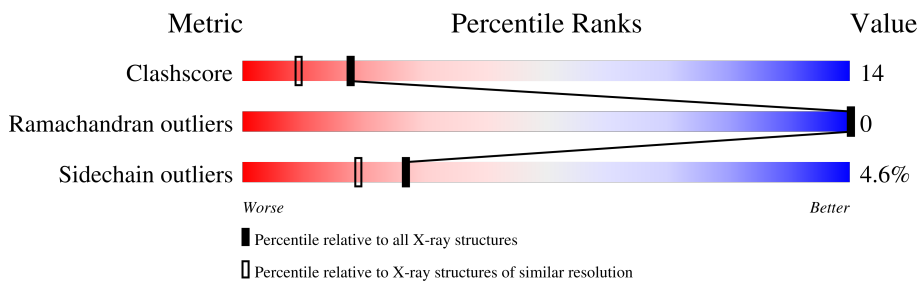
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.06 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	2801 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)





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 ≥ 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	
1	B	200	
1	C	200	
1	D	200	
1	E	200	
1	F	200	
2	M	238	
2	N	238	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain	
2	O	238	 73%	21% ...
2	P	238	 72%	21% ...
2	Q	238	 71%	21% 5% .
2	R	238	 71%	22% ...

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	3HP	M	550	-	-	X	-
5	3HP	R	550	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 22008 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
			Total	C	N	O	S			
1	A	200	1571	993	276	299	3	0	0	0
1	B	200	1571	993	276	299	3	0	0	0
1	C	200	1571	993	276	299	3	0	0	0
1	D	200	1571	993	276	299	3	0	0	0
1	E	200	1571	993	276	299	3	0	0	0
1	F	200	1571	993	276	299	3	0	0	0

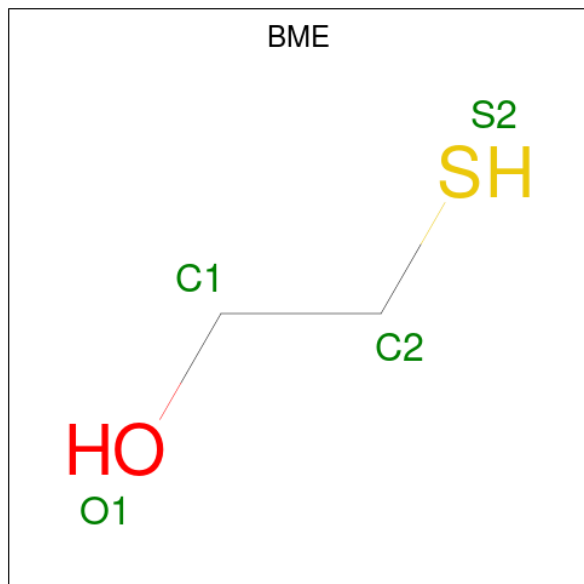
- Molecule 2 is a protein called PROTOCATECHUATE 3,4-DIOXYGENASE.

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

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

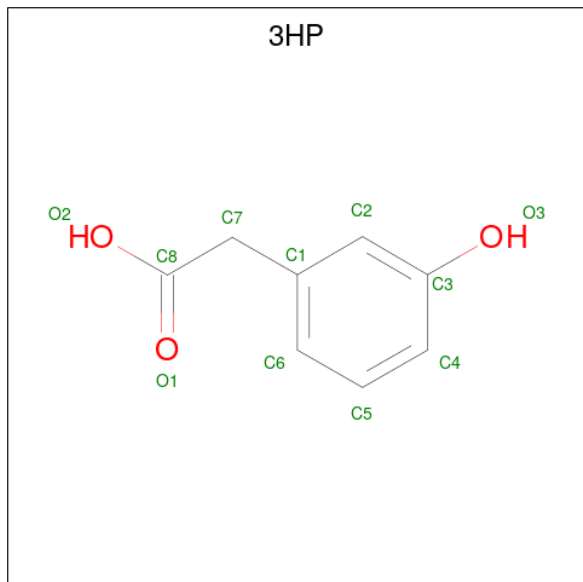
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	M	1	Total Fe 1 1	0	0
3	N	1	Total Fe 1 1	0	0
3	O	1	Total Fe 1 1	0	0
3	P	1	Total Fe 1 1	0	0
3	Q	1	Total Fe 1 1	0	0
3	R	1	Total Fe 1 1	0	0

- Molecule 4 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C₂H₆OS).



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-HYDROXYPHENYLACETATE (three-letter code: 3HP) (formula: $C_8H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	M	1	Total C O 11 8 3	0	0
5	N	1	Total C O 11 8 3	0	0
5	O	1	Total C O 11 8 3	0	0
5	P	1	Total C O 11 8 3	0	0
5	Q	1	Total C O 11 8 3	0	0
5	R	1	Total C O 11 8 3	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	81	Total O 81 81	0	0
6	M	159	Total O 159 159	0	0
6	B	88	Total O 88 88	0	0
6	N	157	Total O 157 157	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	81	Total 81	O 81	0	0
6	O	158	Total 158	O 158	0	0
6	D	80	Total 80	O 80	0	0
6	P	156	Total 156	O 156	0	0
6	E	84	Total 84	O 84	0	0
6	Q	161	Total 161	O 161	0	0
6	F	83	Total 83	O 83	0	0
6	R	158	Total 158	O 158	0	0

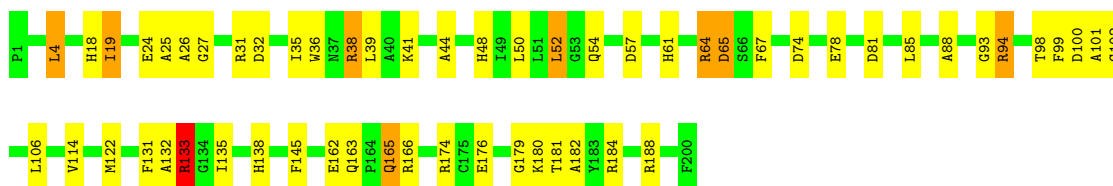
3 Residue-property plots [i](#)

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. 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.

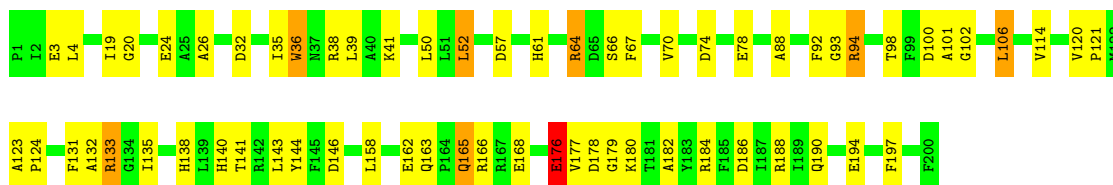
- Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain A: 



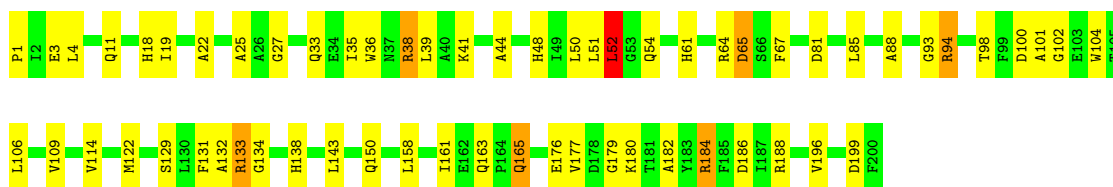
- Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain B: 



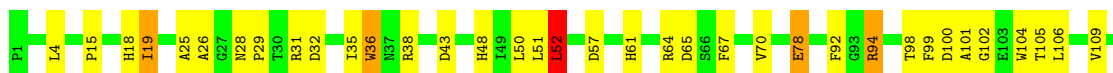
- Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain C: 



- Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain D: 

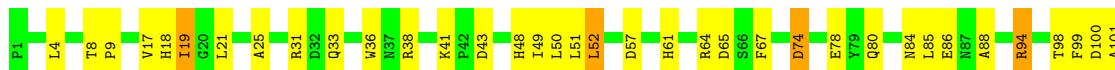




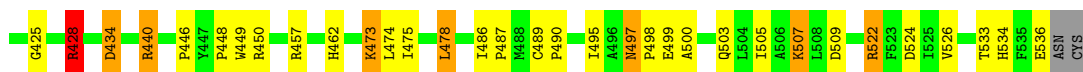
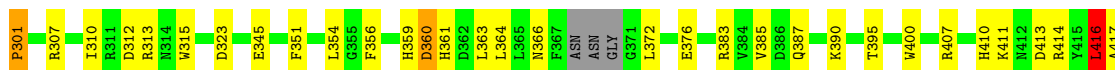
- Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE



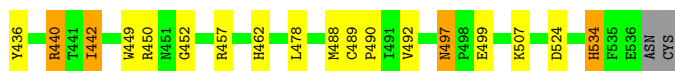
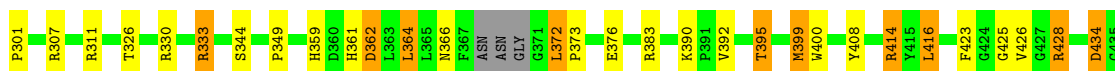
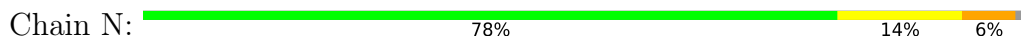
- Molecule 1: PROTOCATECHUATE 3,4-DIOXYGENASE



- Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

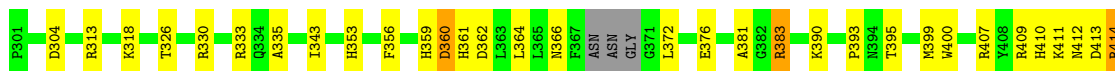


- Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE



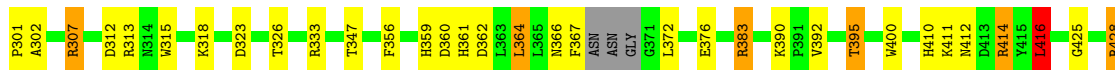
- Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE





• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain P: 72% 21% . . .



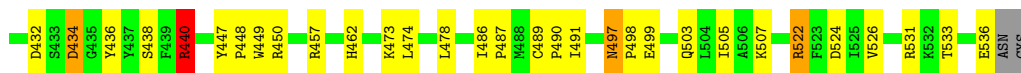
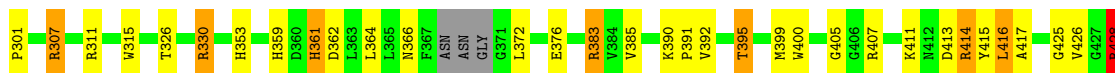
• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain Q: 71% 21% 5% .



• Molecule 2: PROTOCATECHUATE 3,4-DIOXYGENASE

Chain R: 71% 22% . . .



4 Data and refinement statistics

Xtrriage (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, α , β , γ	196.57Å 127.77Å 134.63Å 90.00° 97.70° 90.00°	Depositor
Resolution (Å)	6.00 – 2.06	Depositor
% Data completeness (in resolution range)	79.8 (6.00-2.06)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.169 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	22008	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

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: 3HP, 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	0.95	1/1611 (0.1%)	1.73	32/2195 (1.5%)
1	B	0.98	1/1611 (0.1%)	1.71	32/2195 (1.5%)
1	C	1.02	0/1611	1.56	21/2195 (1.0%)
1	D	1.02	2/1611 (0.1%)	1.80	28/2195 (1.3%)
1	E	1.02	2/1611 (0.1%)	1.70	31/2195 (1.4%)
1	F	1.05	1/1611 (0.1%)	1.71	31/2195 (1.4%)
2	M	1.08	2/1895 (0.1%)	1.64	33/2580 (1.3%)
2	N	1.05	1/1895 (0.1%)	1.66	27/2580 (1.0%)
2	O	1.08	2/1895 (0.1%)	1.63	30/2580 (1.2%)
2	P	1.06	0/1895	1.63	24/2580 (0.9%)
2	Q	1.09	1/1895 (0.1%)	1.54	25/2580 (1.0%)
2	R	1.06	1/1895 (0.1%)	1.65	35/2580 (1.4%)
All	All	1.04	14/21036 (0.1%)	1.66	349/28650 (1.2%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	94	ARG	CD-NE	-7.87	1.33	1.46
1	D	94	ARG	CD-NE	-7.66	1.33	1.46
2	M	428	ARG	CD-NE	-6.24	1.35	1.46
1	E	94	ARG	CD-NE	-5.76	1.36	1.46
2	R	428	ARG	CD-NE	-5.75	1.36	1.46
2	M	345	GLU	CD-OE1	-5.71	1.19	1.25
1	D	133	ARG	CD-NE	-5.62	1.36	1.46
1	B	194	GLU	CD-OE2	-5.38	1.19	1.25
2	O	313	ARG	NE-CZ	5.37	1.40	1.33
1	E	194	GLU	CD-OE2	-5.35	1.19	1.25
2	O	452	GLY	CA-C	5.31	1.60	1.51
1	F	194	GLU	CD-OE2	-5.25	1.19	1.25
2	N	428	ARG	CD-NE	-5.13	1.37	1.46
2	Q	433	SER	CB-OG	5.05	1.48	1.42

All (349) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	133	ARG	CD-NE-CZ	25.85	159.79	123.60
2	N	440	ARG	NE-CZ-NH2	-24.61	107.99	120.30
1	D	94	ARG	NE-CZ-NH1	22.74	131.67	120.30
2	M	440	ARG	NE-CZ-NH2	-21.62	109.49	120.30
2	P	440	ARG	NE-CZ-NH2	-21.16	109.72	120.30
1	D	94	ARG	NE-CZ-NH2	-20.13	110.23	120.30
1	D	94	ARG	CD-NE-CZ	19.03	150.24	123.60
1	A	94	ARG	CD-NE-CZ	18.80	149.92	123.60
2	O	440	ARG	NE-CZ-NH2	-18.63	110.99	120.30
2	R	440	ARG	NE-CZ-NH2	-17.43	111.59	120.30
2	N	311	ARG	CD-NE-CZ	17.25	147.74	123.60
1	B	184	ARG	NE-CZ-NH2	-16.84	111.88	120.30
1	B	94	ARG	NE-CZ-NH1	16.10	128.35	120.30
2	R	428	ARG	NE-CZ-NH1	15.55	128.07	120.30
1	C	94	ARG	NE-CZ-NH1	15.23	127.92	120.30
2	P	440	ARG	NE-CZ-NH1	15.07	127.84	120.30
2	Q	440	ARG	NE-CZ-NH2	-14.88	112.86	120.30
1	E	133	ARG	NE-CZ-NH1	14.86	127.73	120.30
1	F	94	ARG	CD-NE-CZ	14.84	144.38	123.60
1	E	94	ARG	NE-CZ-NH1	14.78	127.69	120.30
2	M	428	ARG	CD-NE-CZ	14.06	143.28	123.60
2	R	428	ARG	CD-NE-CZ	13.90	143.06	123.60
2	P	457	ARG	NE-CZ-NH1	13.89	127.24	120.30
1	B	184	ARG	NE-CZ-NH1	13.74	127.17	120.30
1	F	94	ARG	NE-CZ-NH1	13.50	127.05	120.30
1	A	94	ARG	NE-CZ-NH2	-13.49	113.56	120.30
1	A	94	ARG	NE-CZ-NH1	13.33	126.96	120.30
1	A	38	ARG	NE-CZ-NH2	-13.01	113.80	120.30
1	C	94	ARG	NE-CZ-NH2	-12.90	113.85	120.30
1	F	38	ARG	NE-CZ-NH1	12.82	126.71	120.30
1	F	133	ARG	NE-CZ-NH1	12.77	126.68	120.30
1	F	38	ARG	NE-CZ-NH2	-12.72	113.94	120.30
1	F	142	ARG	NE-CZ-NH1	12.69	126.64	120.30
1	B	38	ARG	NE-CZ-NH2	-12.54	114.03	120.30
2	N	457	ARG	NE-CZ-NH2	-12.27	114.16	120.30
1	D	133	ARG	NE-CZ-NH1	12.24	126.42	120.30
2	N	428	ARG	NE-CZ-NH1	12.21	126.41	120.30
1	B	94	ARG	NE-CZ-NH2	-12.18	114.21	120.30
2	Q	428	ARG	NE-CZ-NH2	-12.13	114.23	120.30
1	E	133	ARG	CD-NE-CZ	12.10	140.54	123.60
1	E	94	ARG	NE-CZ-NH2	-11.99	114.31	120.30
1	A	184	ARG	NE-CZ-NH1	11.93	126.26	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	428	ARG	NE-CZ-NH1	11.91	126.26	120.30
1	C	133	ARG	NE-CZ-NH1	11.82	126.21	120.30
2	O	428	ARG	NE-CZ-NH1	11.62	126.11	120.30
2	Q	428	ARG	NE-CZ-NH1	11.58	126.09	120.30
1	D	94	ARG	CG-CD-NE	11.27	135.46	111.80
1	A	38	ARG	NE-CZ-NH1	11.07	125.83	120.30
2	R	440	ARG	NE-CZ-NH1	11.03	125.81	120.30
1	E	94	ARG	CD-NE-CZ	10.90	138.87	123.60
2	M	414	ARG	NE-CZ-NH1	10.81	125.70	120.30
2	O	428	ARG	CD-NE-CZ	10.78	138.69	123.60
2	P	428	ARG	NE-CZ-NH1	10.73	125.67	120.30
1	A	184	ARG	NE-CZ-NH2	-10.55	115.03	120.30
2	N	440	ARG	NE-CZ-NH1	10.46	125.53	120.30
2	O	333	ARG	NE-CZ-NH2	-10.41	115.09	120.30
1	A	166	ARG	NE-CZ-NH2	-10.40	115.10	120.30
1	E	64	ARG	NE-CZ-NH1	10.32	125.46	120.30
1	B	188	ARG	NE-CZ-NH1	10.23	125.42	120.30
2	P	307	ARG	NE-CZ-NH1	10.14	125.37	120.30
1	F	38	ARG	CD-NE-CZ	10.10	137.74	123.60
1	E	94	ARG	CG-CD-NE	9.99	132.79	111.80
1	C	188	ARG	NE-CZ-NH1	9.75	125.17	120.30
1	C	133	ARG	NE-CZ-NH2	-9.70	115.45	120.30
1	F	133	ARG	CD-NE-CZ	9.62	137.06	123.60
1	E	133	ARG	NE-CZ-NH2	-9.59	115.51	120.30
1	A	94	ARG	CG-CD-NE	9.54	131.82	111.80
1	A	184	ARG	CD-NE-CZ	9.51	136.91	123.60
2	O	531	ARG	NE-CZ-NH1	9.44	125.02	120.30
2	M	428	ARG	NE-CZ-NH2	-9.40	115.60	120.30
1	E	166	ARG	NE-CZ-NH1	9.39	125.00	120.30
2	R	522	ARG	NE-CZ-NH1	-9.18	115.71	120.30
1	F	94	ARG	NE-CZ-NH2	-9.14	115.73	120.30
2	O	383	ARG	NE-CZ-NH2	-9.13	115.74	120.30
2	M	457	ARG	NE-CZ-NH1	9.10	124.85	120.30
1	D	133	ARG	NE-CZ-NH2	-9.02	115.79	120.30
1	E	74	ASP	CB-CG-OD1	9.01	126.41	118.30
2	R	330	ARG	NE-CZ-NH2	-8.83	115.89	120.30
2	M	407	ARG	NE-CZ-NH1	8.76	124.68	120.30
2	Q	377	ARG	NE-CZ-NH1	-8.71	115.94	120.30
2	O	457	ARG	NE-CZ-NH2	-8.71	115.94	120.30
2	Q	457	ARG	NE-CZ-NH1	8.63	124.62	120.30
1	E	38	ARG	NE-CZ-NH2	-8.61	116.00	120.30
2	R	524	ASP	CB-CG-OD1	8.55	126.00	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	450	ARG	NE-CZ-NH1	8.48	124.54	120.30
2	M	323	ASP	CB-CG-OD2	-8.41	110.73	118.30
2	N	311	ARG	NE-CZ-NH2	-8.37	116.11	120.30
2	O	434	ASP	CB-CG-OD2	-8.35	110.79	118.30
2	O	428	ARG	NE-CZ-NH2	-8.30	116.15	120.30
1	C	184	ARG	NE-CZ-NH1	8.29	124.45	120.30
1	F	188	ARG	NE-CZ-NH2	-8.26	116.17	120.30
1	A	188	ARG	NE-CZ-NH2	-8.21	116.19	120.30
1	A	81	ASP	CB-CG-OD1	8.16	125.65	118.30
1	E	38	ARG	NE-CZ-NH1	8.15	124.38	120.30
2	N	307	ARG	NE-CZ-NH1	8.14	124.37	120.30
1	A	188	ARG	NE-CZ-NH1	8.12	124.36	120.30
2	Q	450	ARG	NE-CZ-NH1	8.11	124.36	120.30
1	E	166	ARG	NE-CZ-NH2	-8.11	116.25	120.30
2	N	428	ARG	NE-CZ-NH2	-8.06	116.27	120.30
1	F	142	ARG	NE-CZ-NH2	-8.04	116.28	120.30
2	R	457	ARG	NE-CZ-NH2	-8.04	116.28	120.30
1	B	188	ARG	NE-CZ-NH2	-8.02	116.29	120.30
1	F	94	ARG	CG-CD-NE	8.01	128.63	111.80
1	D	65	ASP	CB-CG-OD1	7.98	125.48	118.30
2	N	414	ARG	NE-CZ-NH1	7.97	124.29	120.30
2	N	524	ASP	CB-CG-OD2	-7.97	111.13	118.30
2	R	522	ARG	NE-CZ-NH2	7.97	124.28	120.30
1	B	133	ARG	NE-CZ-NH1	7.94	124.27	120.30
1	D	167	ARG	NE-CZ-NH1	7.93	124.27	120.30
1	B	38	ARG	NE-CZ-NH1	7.93	124.26	120.30
2	R	428	ARG	NE-CZ-NH2	-7.92	116.34	120.30
1	F	133	ARG	NE-CZ-NH2	-7.89	116.35	120.30
2	R	531	ARG	NE-CZ-NH1	7.83	124.22	120.30
1	B	133	ARG	CD-NE-CZ	7.81	134.54	123.60
1	C	186	ASP	CB-CG-OD1	7.79	125.31	118.30
2	M	440	ARG	NH1-CZ-NH2	7.75	127.93	119.40
2	N	333	ARG	NE-CZ-NH2	-7.73	116.44	120.30
2	O	450	ARG	NE-CZ-NH1	7.73	124.16	120.30
1	A	64	ARG	NE-CZ-NH1	-7.55	116.52	120.30
2	Q	407	ARG	NE-CZ-NH1	7.55	124.08	120.30
2	O	457	ARG	NE-CZ-NH1	7.52	124.06	120.30
2	M	450	ARG	NE-CZ-NH1	7.50	124.05	120.30
1	D	57	ASP	CB-CG-OD1	7.47	125.02	118.30
1	F	174	ARG	CD-NE-CZ	-7.46	113.16	123.60
1	F	38	ARG	CA-CB-CG	7.45	129.78	113.40
2	R	428	ARG	CG-CD-NE	7.45	127.44	111.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	428	ARG	CG-CD-NE	7.45	127.44	111.80
2	P	307	ARG	NE-CZ-NH2	-7.36	116.62	120.30
1	E	74	ASP	CB-CG-OD2	-7.36	111.67	118.30
1	C	81	ASP	CB-CG-OD1	7.34	124.91	118.30
2	P	457	ARG	NE-CZ-NH2	-7.33	116.64	120.30
2	N	307	ARG	NE-CZ-NH2	-7.32	116.64	120.30
1	A	133	ARG	NE-CZ-NH2	7.29	123.95	120.30
2	M	323	ASP	CB-CG-OD1	7.29	124.86	118.30
2	O	440	ARG	NH1-CZ-NH2	7.28	127.40	119.40
2	R	524	ASP	CB-CG-OD2	-7.22	111.80	118.30
2	P	434	ASP	CB-CG-OD1	-7.21	111.81	118.30
2	M	414	ARG	NE-CZ-NH2	-7.17	116.72	120.30
1	B	166	ARG	NE-CZ-NH2	-7.17	116.72	120.30
2	P	522	ARG	NE-CZ-NH1	-7.14	116.73	120.30
2	P	432	ASP	CB-CG-OD1	7.13	124.72	118.30
2	P	457	ARG	CD-NE-CZ	7.13	133.59	123.60
2	R	307	ARG	NE-CZ-NH1	7.12	123.86	120.30
2	P	524	ASP	CB-CG-OD1	7.11	124.70	118.30
1	D	158	LEU	CB-CA-C	7.10	123.69	110.20
1	D	184	ARG	NE-CZ-NH1	7.09	123.84	120.30
2	R	311	ARG	NE-CZ-NH2	-7.07	116.76	120.30
1	E	142	ARG	NE-CZ-NH2	-7.02	116.79	120.30
2	Q	312	ASP	CB-CG-OD1	7.02	124.62	118.30
1	E	65	ASP	CB-CG-OD1	7.00	124.61	118.30
1	B	176	GLU	CB-CG-CD	7.00	133.11	114.20
2	O	313	ARG	NE-CZ-NH2	-6.97	116.81	120.30
2	Q	457	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	B	178	ASP	CB-CG-OD2	6.95	124.56	118.30
1	C	133	ARG	CD-NE-CZ	6.95	133.33	123.60
2	R	383	ARG	NE-CZ-NH2	-6.95	116.83	120.30
2	R	414	ARG	NE-CZ-NH2	-6.93	116.83	120.30
1	E	188	ARG	NE-CZ-NH1	6.93	123.76	120.30
2	O	450	ARG	NE-CZ-NH2	-6.90	116.85	120.30
2	R	311	ARG	CD-NE-CZ	6.87	133.22	123.60
2	P	428	ARG	CG-CD-NE	6.84	126.16	111.80
1	F	74	ASP	CB-CG-OD1	6.82	124.44	118.30
2	R	376	GLU	OE1-CD-OE2	6.82	131.48	123.30
1	B	57	ASP	CB-CG-OD2	-6.80	112.18	118.30
1	B	94	ARG	CD-NE-CZ	6.80	133.12	123.60
2	P	428	ARG	NE-CZ-NH2	-6.79	116.90	120.30
1	A	81	ASP	CB-CG-OD2	-6.79	112.19	118.30
1	B	186	ASP	CB-CG-OD2	-6.75	112.22	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	38	ARG	CD-NE-CZ	-6.73	114.17	123.60
1	F	158	LEU	CB-CA-C	6.73	122.98	110.20
1	C	52	LEU	CB-CA-C	6.73	122.98	110.20
2	R	311	ARG	NE-CZ-NH1	6.72	123.66	120.30
2	M	383	ARG	NE-CZ-NH1	-6.71	116.94	120.30
1	B	52	LEU	CA-CB-CG	6.71	130.74	115.30
2	O	353	HIS	CA-CB-CG	-6.71	102.19	113.60
2	O	409	ARG	NE-CZ-NH2	6.69	123.65	120.30
1	E	186	ASP	CB-CG-OD1	6.69	124.32	118.30
1	C	11	GLN	N-CA-CB	6.68	122.63	110.60
2	R	531	ARG	NE-CZ-NH2	-6.67	116.96	120.30
1	D	188	ARG	NE-CZ-NH2	-6.65	116.97	120.30
1	A	36	TRP	CB-CA-C	6.65	123.69	110.40
2	N	434	ASP	CB-CG-OD2	-6.64	112.32	118.30
2	M	312	ASP	CB-CG-OD2	-6.62	112.34	118.30
2	Q	434	ASP	CB-CG-OD2	-6.61	112.35	118.30
2	Q	432	ASP	CB-CG-OD1	6.61	124.25	118.30
2	Q	376	GLU	OE1-CD-OE2	6.60	131.22	123.30
1	A	166	ARG	NE-CZ-NH1	6.57	123.58	120.30
1	C	94	ARG	CD-NE-CZ	6.55	132.78	123.60
2	O	330	ARG	NE-CZ-NH2	-6.55	117.02	120.30
1	B	176	GLU	OE1-CD-OE2	-6.53	115.47	123.30
2	M	434	ASP	CB-CG-OD2	-6.48	112.47	118.30
1	F	166	ARG	NE-CZ-NH1	6.47	123.54	120.30
2	Q	440	ARG	NE-CZ-NH1	6.45	123.53	120.30
2	M	312	ASP	CB-CG-OD1	6.43	124.09	118.30
1	E	94	ARG	CB-CG-CD	6.43	128.32	111.60
2	O	383	ARG	NE-CZ-NH1	6.37	123.48	120.30
1	C	38	ARG	CD-NE-CZ	-6.36	114.70	123.60
1	F	52	LEU	CA-CB-CG	6.35	129.90	115.30
2	R	432	ASP	CB-CG-OD2	-6.35	112.59	118.30
2	P	383	ARG	NE-CZ-NH1	-6.34	117.13	120.30
1	B	94	ARG	CG-CD-NE	6.33	125.10	111.80
2	R	414	ARG	NE-CZ-NH1	6.33	123.46	120.30
2	N	311	ARG	NE-CZ-NH1	6.32	123.46	120.30
2	M	522	ARG	NE-CZ-NH1	-6.31	117.14	120.30
2	M	313	ARG	NE-CZ-NH1	6.30	123.45	120.30
2	R	434	ASP	CB-CG-OD2	-6.29	112.64	118.30
1	E	81	ASP	CB-CG-OD1	6.29	123.96	118.30
2	N	440	ARG	NH1-CZ-NH2	6.28	126.30	119.40
2	O	360	ASP	CB-CG-OD2	-6.28	112.65	118.30
2	P	312	ASP	CB-CG-OD2	-6.27	112.66	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	407	ARG	NE-CZ-NH2	-6.27	117.17	120.30
1	D	57	ASP	CB-CG-OD2	-6.23	112.69	118.30
2	R	361	HIS	CA-CB-CG	-6.22	103.02	113.60
1	A	52	LEU	CB-CA-C	6.22	122.01	110.20
2	Q	432	ASP	CB-CG-OD2	-6.22	112.70	118.30
2	R	407	ARG	NE-CZ-NH1	6.21	123.40	120.30
2	O	420	ASP	CB-CG-OD1	6.20	123.88	118.30
1	A	31	ARG	NE-CZ-NH2	-6.17	117.21	120.30
2	R	457	ARG	CA-CB-CG	6.15	126.94	113.40
1	E	52	LEU	CB-CA-C	6.14	121.87	110.20
2	M	413	ASP	CB-CG-OD1	6.14	123.83	118.30
1	A	65	ASP	CB-CG-OD1	6.05	123.74	118.30
2	P	524	ASP	CB-CG-OD2	-6.05	112.86	118.30
1	D	188	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	B	176	GLU	CG-CD-OE1	6.01	130.33	118.30
1	F	57	ASP	CB-CG-OD2	-5.99	112.91	118.30
2	O	522	ARG	NE-CZ-NH2	5.96	123.28	120.30
2	M	524	ASP	CB-CG-OD1	5.95	123.66	118.30
2	M	428	ARG	CG-CD-NE	5.94	124.27	111.80
2	R	353	HIS	CA-CB-CG	-5.94	103.50	113.60
1	E	78	GLU	CG-CD-OE2	-5.93	106.44	118.30
2	R	450	ARG	NE-CZ-NH2	-5.93	117.34	120.30
1	F	188	ARG	NE-CZ-NH1	5.92	123.26	120.30
2	M	457	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	A	32	ASP	CB-CG-OD1	5.88	123.59	118.30
1	D	146	ASP	CB-CG-OD2	-5.86	113.03	118.30
1	D	52	LEU	CB-CA-C	5.86	121.33	110.20
2	O	517	ASP	CB-CG-OD1	5.85	123.57	118.30
2	P	440	ARG	CD-NE-CZ	5.84	131.77	123.60
2	N	457	ARG	NE-CZ-NH1	5.84	123.22	120.30
2	Q	450	ARG	NE-CZ-NH2	-5.83	117.38	120.30
2	N	434	ASP	OD1-CG-OD2	5.82	134.35	123.30
2	N	434	ASP	CB-CG-OD1	-5.81	113.07	118.30
1	F	36	TRP	CB-CA-C	5.80	122.00	110.40
1	E	36	TRP	CB-CA-C	5.80	122.00	110.40
2	Q	524	ASP	CB-CG-OD2	-5.79	113.08	118.30
2	N	450	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	C	186	ASP	CB-CG-OD2	-5.79	113.09	118.30
1	A	31	ARG	NE-CZ-NH1	5.78	123.19	120.30
2	Q	312	ASP	CB-CG-OD2	-5.70	113.17	118.30
1	D	94	ARG	CB-CG-CD	5.69	126.40	111.60
2	M	524	ASP	CB-CG-OD2	-5.66	113.21	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	452	GLY	N-CA-C	-5.65	98.98	113.10
2	Q	428	ARG	CG-CD-NE	5.64	123.65	111.80
1	F	52	LEU	CB-CA-C	5.64	120.92	110.20
2	O	416	LEU	CB-CA-C	5.64	120.91	110.20
2	O	452	GLY	N-CA-C	-5.63	99.02	113.10
1	D	184	ARG	NE-CZ-NH2	-5.63	117.48	120.30
2	R	330	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	D	36	TRP	CB-CA-C	5.62	121.63	110.40
1	A	174	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	E	158	LEU	CB-CA-C	5.61	120.86	110.20
2	R	376	GLU	CG-CD-OE2	-5.61	107.08	118.30
1	A	52	LEU	CA-CB-CG	5.60	128.19	115.30
1	A	74	ASP	CB-CG-OD2	-5.59	113.27	118.30
2	M	522	ARG	CD-NE-CZ	-5.59	115.78	123.60
1	D	166	ARG	NE-CZ-NH2	-5.58	117.51	120.30
2	M	417	ALA	CB-CA-C	5.58	118.47	110.10
1	A	74	ASP	CB-CG-OD1	5.57	123.31	118.30
1	B	36	TRP	CB-CA-C	5.55	121.50	110.40
2	N	428	ARG	CD-NE-CZ	5.53	131.34	123.60
2	O	414	ARG	NE-CZ-NH1	-5.53	117.54	120.30
2	N	524	ASP	CB-CG-OD1	5.52	123.27	118.30
1	D	25	ALA	CB-CA-C	5.52	118.39	110.10
2	N	440	ARG	CB-CG-CD	-5.51	97.26	111.60
1	B	24	GLU	CA-CB-CG	5.51	125.52	113.40
2	R	434	ASP	CA-CB-CG	-5.50	101.29	113.40
2	M	383	ARG	NH1-CZ-NH2	5.49	125.44	119.40
1	E	174	ARG	NE-CZ-NH1	-5.49	117.56	120.30
1	B	66	SER	N-CA-CB	5.47	118.71	110.50
1	A	64	ARG	CD-NE-CZ	-5.46	115.95	123.60
1	F	57	ASP	CB-CG-OD1	5.46	123.21	118.30
1	D	186	ASP	CB-CG-OD1	5.45	123.20	118.30
1	E	52	LEU	CA-CB-CG	5.44	127.80	115.30
2	O	407	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	F	181	THR	N-CA-CB	5.43	120.62	110.30
2	M	360	ASP	CB-CG-OD1	5.42	123.18	118.30
2	Q	531	ARG	NE-CZ-NH1	5.41	123.01	120.30
2	P	416	LEU	CB-CA-C	5.39	120.45	110.20
2	O	335	ALA	CB-CA-C	-5.39	102.02	110.10
2	P	312	ASP	CB-CG-OD1	5.38	123.14	118.30
2	P	333	ARG	NE-CZ-NH1	-5.37	117.61	120.30
2	M	383	ARG	NE-CZ-NH2	-5.37	117.62	120.30
1	D	78	GLU	OE1-CD-OE2	5.37	129.74	123.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	94	ARG	CB-CG-CD	5.37	125.55	111.60
1	C	65	ASP	CB-CG-OD1	5.37	123.13	118.30
1	D	146	ASP	CB-CG-OD1	5.37	123.13	118.30
1	F	74	ASP	CB-CG-OD2	-5.36	113.47	118.30
1	B	64	ARG	CD-NE-CZ	-5.35	116.11	123.60
1	D	186	ASP	CB-CG-OD2	-5.35	113.48	118.30
2	M	509	ASP	CB-CG-OD1	5.35	123.12	118.30
1	F	65	ASP	CB-CG-OD1	5.35	123.11	118.30
2	O	414	ARG	CD-NE-CZ	-5.34	116.12	123.60
2	Q	377	ARG	NE-CZ-NH2	5.33	122.97	120.30
2	R	438	SER	N-CA-CB	5.31	118.47	110.50
1	F	94	ARG	CB-CG-CD	5.30	125.39	111.60
2	Q	499	GLU	CG-CD-OE1	5.30	128.90	118.30
2	N	383	ARG	NE-CZ-NH2	-5.30	117.65	120.30
2	Q	452	GLY	N-CA-C	-5.29	99.87	113.10
1	C	129	SER	N-CA-CB	5.29	118.43	110.50
1	D	43	ASP	CB-CG-OD1	-5.29	113.54	118.30
1	B	162	GLU	OE1-CD-OE2	5.28	129.64	123.30
1	B	186	ASP	CB-CG-OD1	5.27	123.05	118.30
2	Q	416	LEU	CB-CA-C	5.27	120.21	110.20
1	E	167	ARG	NE-CZ-NH2	5.26	122.93	120.30
1	B	168	GLU	CG-CD-OE1	5.25	128.81	118.30
1	E	146	ASP	CB-CG-OD1	5.25	123.03	118.30
1	E	13	ALA	CB-CA-C	5.24	117.96	110.10
1	B	158	LEU	CB-CA-C	5.22	120.12	110.20
2	N	362	ASP	CB-CG-OD1	5.22	123.00	118.30
1	B	146	ASP	CB-CG-OD1	5.21	122.99	118.30
1	B	74	ASP	CB-CG-OD1	5.17	122.96	118.30
1	F	186	ASP	CB-CG-OD1	5.17	122.96	118.30
1	B	57	ASP	CB-CG-OD1	5.16	122.94	118.30
1	E	57	ASP	CB-CG-OD2	-5.16	113.66	118.30
2	Q	428	ARG	CD-NE-CZ	5.15	130.81	123.60
2	O	333	ARG	NH1-CZ-NH2	5.15	125.06	119.40
1	F	174	ARG	NE-CZ-NH2	-5.14	117.73	120.30
2	P	452	GLY	N-CA-C	-5.14	100.25	113.10
2	N	416	LEU	CB-CA-C	5.13	119.94	110.20
2	M	450	ARG	CD-NE-CZ	5.12	130.76	123.60
1	A	174	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	C	188	ARG	NE-CZ-NH2	-5.11	117.74	120.30
1	E	186	ASP	CB-CG-OD2	-5.10	113.71	118.30
1	C	158	LEU	CB-CA-C	5.10	119.89	110.20
2	M	440	ARG	CB-CG-CD	-5.08	98.39	111.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	57	ASP	CB-CG-OD1	5.08	122.87	118.30
2	Q	376	GLU	CG-CD-OE2	-5.07	108.15	118.30
1	C	25	ALA	CB-CA-C	5.06	117.69	110.10
1	F	43	ASP	CB-CG-OD1	-5.05	113.76	118.30
2	M	411	LYS	CB-CA-C	-5.05	100.31	110.40
2	P	323	ASP	CB-CG-OD1	5.04	122.84	118.30
1	C	36	TRP	CB-CA-C	5.04	120.48	110.40
1	B	52	LEU	CB-CA-C	5.04	119.77	110.20
1	A	162	GLU	CA-CB-CG	5.02	124.45	113.40
2	M	416	LEU	CA-CB-CG	5.01	126.82	115.30
1	C	199	ASP	CB-CG-OD2	5.01	122.81	118.30
2	O	434	ASP	CA-CB-CG	-5.00	102.39	113.40
2	P	367	PHE	CA-C-O	-5.00	109.59	120.10

There are no chirality outliers.

There are no planarity outliers.

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	1571	0	1499	48	0
1	B	1571	0	1499	43	0
1	C	1571	0	1499	46	0
1	D	1571	0	1499	46	0
1	E	1571	0	1499	55	0
1	F	1571	0	1499	56	0
2	M	1840	0	1792	50	0
2	N	1840	0	1792	35	0
2	O	1840	0	1792	46	0
2	P	1840	0	1792	53	0
2	Q	1840	0	1792	51	0
2	R	1840	0	1792	54	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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	1	0
4	O	4	0	5	1	0
4	P	4	0	5	0	0
4	Q	4	0	5	3	0
4	R	4	0	5	1	0
5	M	11	0	6	4	0
5	N	11	0	6	3	0
5	O	11	0	6	3	0
5	P	11	0	6	3	0
5	Q	11	0	6	3	0
5	R	11	0	6	4	0
6	A	81	0	0	2	0
6	B	88	0	0	2	0
6	C	81	0	0	0	0
6	D	80	0	0	1	0
6	E	84	0	0	0	0
6	F	83	0	0	1	0
6	M	159	0	0	3	0
6	N	157	0	0	3	0
6	O	158	0	0	5	0
6	P	156	0	0	3	0
6	Q	161	0	0	2	0
6	R	158	0	0	3	0
All	All	22008	0	19812	549	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 14.

All (549) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:165:GLN:H	1:E:165:GLN:NE2	1.41	1.17
1:B:165:GLN:H	1:B:165:GLN:NE2	1.43	1.14
1:E:165:GLN:HE21	1:E:165:GLN:N	1.45	1.13
2:P:364:LEU:HD22	2:P:440:ARG:HD3	1.16	1.11
1:F:163:GLN:HB3	1:F:165:GLN:HE22	1.13	1.10
1:A:98:THR:HB	1:A:100:ASP:OD1	1.56	1.06
2:R:497:ASN:ND2	2:R:499:GLU:H	1.58	1.01

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:41:LYS:HD2	1:E:88:ALA:HA	1.43	0.99
1:C:64:ARG:NH1	1:C:100:ASP:O	1.97	0.97
1:A:163:GLN:HB3	1:A:165:GLN:NE2	1.81	0.95
1:D:64:ARG:NH1	1:D:100:ASP:O	1.99	0.95
1:F:163:GLN:HB3	1:F:165:GLN:NE2	1.80	0.95
1:B:165:GLN:H	1:B:165:GLN:HE21	1.00	0.95
2:R:361:HIS:H	2:R:361:HIS:CD2	1.80	0.95
2:P:364:LEU:CD2	2:P:440:ARG:HD3	1.97	0.93
1:D:165:GLN:H	1:D:165:GLN:HE21	1.04	0.93
2:R:497:ASN:HD22	2:R:499:GLU:H	1.17	0.93
1:C:163:GLN:HB3	1:C:165:GLN:NE2	1.85	0.92
1:E:98:THR:HB	1:E:100:ASP:OD1	1.69	0.92
2:R:505:ILE:HG22	2:R:507:LYS:HE3	1.52	0.91
1:B:165:GLN:HE21	1:B:165:GLN:N	1.68	0.91
1:D:165:GLN:H	1:D:165:GLN:NE2	1.68	0.90
1:A:163:GLN:HB3	1:A:165:GLN:HE22	1.33	0.90
1:E:64:ARG:NH1	1:E:100:ASP:O	2.05	0.90
2:M:497:ASN:ND2	2:M:499:GLU:H	1.70	0.90
1:F:64:ARG:NH1	1:F:100:ASP:O	2.06	0.89
2:M:497:ASN:HD22	2:M:499:GLU:H	1.19	0.88
1:B:67:PHE:HZ	1:B:94:ARG:HD2	1.37	0.87
1:F:98:THR:OG1	1:F:102:GLY:N	2.09	0.86
1:B:98:THR:HB	1:B:100:ASP:OD1	1.75	0.85
1:F:98:THR:HB	1:F:100:ASP:OD1	1.78	0.84
2:R:361:HIS:H	2:R:361:HIS:HD2	1.19	0.84
2:R:462:HIS:HE1	5:R:550:3HP:H4	1.40	0.84
1:A:176:GLU:OE2	1:A:179:GLY:HA2	1.78	0.84
1:D:98:THR:OG1	1:D:102:GLY:N	2.14	0.80
1:E:168:GLU:HA	1:E:171:ILE:HD12	1.64	0.80
1:C:33:GLN:HG2	1:C:85:LEU:HD12	1.64	0.79
1:D:165:GLN:HE21	1:D:165:GLN:N	1.80	0.79
2:Q:361:HIS:CD2	2:Q:361:HIS:H	2.00	0.79
1:F:176:GLU:HG2	1:F:179:GLY:HA2	1.64	0.79
1:A:67:PHE:HZ	1:A:94:ARG:HD2	1.48	0.78
2:O:497:ASN:HD22	2:O:499:GLU:H	1.30	0.78
2:Q:390:LYS:HD2	6:Q:1040:HOH:O	1.83	0.78
2:P:497:ASN:HD22	2:P:499:GLU:H	1.32	0.77
1:E:51:LEU:HD12	1:E:106:LEU:HD23	1.64	0.77
1:C:67:PHE:HZ	1:C:94:ARG:HD2	1.49	0.77
1:A:64:ARG:NH1	1:A:100:ASP:O	2.18	0.77
2:N:390:LYS:HD3	6:N:645:HOH:O	1.85	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:ARG:NH1	1:B:100:ASP:O	2.18	0.76
2:O:497:ASN:ND2	2:O:499:GLU:H	1.84	0.76
1:F:177:VAL:O	1:F:180:LYS:HB3	1.86	0.76
2:R:361:HIS:CD2	2:R:361:HIS:N	2.54	0.75
1:E:67:PHE:HZ	1:E:94:ARG:HD2	1.50	0.75
2:N:497:ASN:HD22	2:N:499:GLU:H	1.36	0.74
2:Q:497:ASN:ND2	2:Q:499:GLU:H	1.86	0.73
1:B:67:PHE:CZ	1:B:94:ARG:HD2	2.23	0.73
2:P:313:ARG:O	2:P:318:LYS:HE3	1.89	0.73
2:P:361:HIS:H	2:P:361:HIS:CD2	2.06	0.73
1:F:33:GLN:HG2	1:F:85:LEU:HD12	1.69	0.73
2:N:390:LYS:HE2	6:N:721:HOH:O	1.88	0.72
1:C:98:THR:OG1	1:C:102:GLY:N	2.21	0.72
1:D:177:VAL:O	1:D:180:LYS:HB3	1.89	0.72
1:F:163:GLN:CB	1:F:165:GLN:HE22	2.00	0.72
1:B:19:ILE:HG22	1:B:26:ALA:HB1	1.72	0.72
2:P:390:LYS:HE2	6:P:727:HOH:O	1.90	0.72
2:Q:361:HIS:H	2:Q:361:HIS:HD2	1.37	0.71
2:P:364:LEU:HD22	2:P:440:ARG:CD	2.08	0.71
2:Q:497:ASN:ND2	2:Q:499:GLU:OE1	2.22	0.71
1:B:165:GLN:NE2	1:B:165:GLN:N	2.28	0.71
1:C:35:ILE:HG22	1:C:94:ARG:HG3	1.73	0.71
1:A:67:PHE:CZ	1:A:94:ARG:HD2	2.25	0.70
1:A:98:THR:OG1	1:A:102:GLY:N	2.24	0.70
1:D:176:GLU:HG2	1:D:179:GLY:HA2	1.73	0.70
2:P:462:HIS:HE1	5:P:550:3HP:H4	1.56	0.70
1:E:163:GLN:HB3	1:E:165:GLN:HE22	1.57	0.70
1:B:163:GLN:HB3	1:B:165:GLN:NE2	2.06	0.70
1:F:100:ASP:CG	1:F:101:ALA:H	1.96	0.69
2:R:497:ASN:ND2	2:R:499:GLU:OE1	2.26	0.69
1:F:78:GLU:HG2	2:R:301:PRO:HG2	1.74	0.69
2:R:473:LYS:HD2	2:R:474:LEU:N	2.08	0.69
2:Q:449:TRP:CE3	5:Q:550:3HP:H71	2.27	0.69
1:F:51:LEU:HD12	1:F:106:LEU:HD23	1.75	0.69
2:R:497:ASN:ND2	2:R:499:GLU:N	2.38	0.69
1:E:98:THR:OG1	1:E:102:GLY:N	2.24	0.68
2:N:449:TRP:CE3	5:N:550:3HP:H71	2.28	0.68
1:D:98:THR:HB	1:D:100:ASP:OD1	1.94	0.68
2:R:462:HIS:CE1	5:R:550:3HP:H4	2.26	0.68
1:E:163:GLN:HB3	1:E:165:GLN:NE2	2.08	0.68
1:A:78:GLU:OE1	6:A:239:HOH:O	2.12	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:GLU:HG3	1:A:180:LYS:O	1.94	0.67
2:N:361:HIS:CD2	2:N:361:HIS:H	2.11	0.67
1:C:165:GLN:NE2	1:C:165:GLN:H	1.92	0.67
2:M:449:TRP:CE3	5:M:550:3HP:H71	2.29	0.67
1:C:67:PHE:CZ	1:C:94:ARG:HD2	2.30	0.67
1:C:163:GLN:HB3	1:C:165:GLN:HE22	1.60	0.67
2:R:497:ASN:HD22	2:R:499:GLU:N	1.93	0.66
2:N:497:ASN:ND2	2:N:499:GLU:H	1.94	0.66
2:M:361:HIS:H	2:M:361:HIS:CD2	2.11	0.66
1:A:100:ASP:CG	1:A:101:ALA:H	1.99	0.66
1:D:176:GLU:HA	1:D:180:LYS:O	1.97	0.65
2:P:360:ASP:OD2	2:P:428:ARG:HD2	1.97	0.65
1:B:176:GLU:HG3	1:B:180:LYS:O	1.97	0.65
5:O:550:3HP:O2	6:O:754:HOH:O	2.13	0.65
2:P:449:TRP:CE3	5:P:550:3HP:H71	2.32	0.65
1:E:180:LYS:HG3	1:E:181:THR:N	2.10	0.65
2:Q:315:TRP:HZ2	2:Q:503:GLN:HE21	1.43	0.65
2:O:361:HIS:H	2:O:361:HIS:CD2	2.16	0.64
1:D:18:HIS:CE1	1:D:99:PHE:HE1	2.15	0.64
2:P:497:ASN:ND2	2:P:499:GLU:H	1.94	0.64
1:F:165:GLN:CD	1:F:165:GLN:H	1.99	0.64
2:P:416:LEU:C	2:P:416:LEU:HD23	2.19	0.64
1:B:41:LYS:HD2	1:B:88:ALA:HA	1.79	0.63
1:A:176:GLU:HA	1:A:180:LYS:O	1.97	0.63
2:Q:497:ASN:HD22	2:Q:499:GLU:H	1.43	0.63
1:A:163:GLN:CB	1:A:165:GLN:HE22	2.09	0.63
5:N:550:3HP:O2	6:N:747:HOH:O	2.16	0.63
1:E:143:LEU:HD23	1:E:143:LEU:C	2.18	0.63
2:R:315:TRP:HZ2	2:R:503:GLN:HE21	1.46	0.63
2:R:307:ARG:NE	2:R:536:GLU:OE2	2.31	0.63
2:R:497:ASN:HD22	2:R:498:PRO:N	1.96	0.63
1:A:18:HIS:CE1	1:A:99:PHE:HE1	2.17	0.62
1:A:41:LYS:HD2	1:A:88:ALA:HA	1.81	0.62
1:B:3:GLU:HA	1:B:3:GLU:OE1	2.00	0.62
2:O:413:ASP:O	2:O:414:ARG:HD2	1.99	0.62
1:F:18:HIS:CE1	1:F:99:PHE:HE1	2.18	0.62
2:R:400:TRP:HA	2:R:425:GLY:O	2.00	0.62
2:M:446:PRO:HD2	2:P:376:GLU:HG2	1.82	0.62
1:E:67:PHE:CZ	1:E:94:ARG:HD2	2.34	0.62
2:Q:413:ASP:O	2:Q:414:ARG:NH1	2.33	0.61
2:R:497:ASN:HD22	2:R:497:ASN:C	2.02	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:497:ASN:ND2	2:N:499:GLU:HB2	2.15	0.61
1:F:176:GLU:HG3	1:F:180:LYS:N	2.15	0.61
1:D:100:ASP:CG	1:D:101:ALA:H	2.03	0.61
2:Q:376:GLU:O	2:Q:442:ILE:HA	2.00	0.61
1:C:100:ASP:CG	1:C:101:ALA:H	2.02	0.61
2:O:413:ASP:C	2:O:414:ARG:HD2	2.21	0.61
2:O:434:ASP:HB3	2:O:436:TYR:CD2	2.35	0.61
1:D:163:GLN:HB3	1:D:165:GLN:NE2	2.14	0.60
1:D:67:PHE:CZ	1:D:94:ARG:HD2	2.36	0.60
2:N:359:HIS:O	2:N:366:ASN:HB3	2.02	0.60
1:C:54:GLN:HG3	1:C:184:ARG:NH2	2.16	0.60
1:D:18:HIS:CE1	1:D:99:PHE:CE1	2.90	0.60
2:Q:462:HIS:HE1	5:Q:550:3HP:H4	1.66	0.60
1:C:98:THR:HB	1:C:100:ASP:OD1	2.01	0.60
2:O:364:LEU:HD22	2:O:440:ARG:HD3	1.82	0.60
2:N:361:HIS:H	2:N:361:HIS:HD2	1.48	0.60
2:M:462:HIS:HE1	5:M:550:3HP:H4	1.65	0.60
2:Q:497:ASN:HD22	2:Q:497:ASN:C	2.06	0.60
1:F:176:GLU:HA	1:F:180:LYS:O	2.02	0.60
2:P:356:PHE:HD1	2:P:428:ARG:HD3	1.67	0.60
1:D:67:PHE:HZ	1:D:94:ARG:HD2	1.66	0.59
2:Q:361:HIS:CG	4:Q:601:BME:H21	2.38	0.59
1:A:165:GLN:CD	1:A:165:GLN:H	2.04	0.59
2:N:488:MET:CE	1:C:1:PRO:HG3	2.32	0.59
1:E:41:LYS:HE3	1:E:87:ASN:O	2.03	0.59
2:M:361:HIS:H	2:M:361:HIS:HD2	1.50	0.59
1:D:168:GLU:HA	1:D:171:ILE:HD12	1.85	0.58
1:F:18:HIS:CE1	1:F:99:PHE:CE1	2.90	0.58
1:E:65:ASP:OD2	1:E:133:ARG:HD3	2.03	0.58
2:P:361:HIS:H	2:P:361:HIS:HD2	1.49	0.58
1:E:168:GLU:HA	1:E:171:ILE:CD1	2.32	0.58
1:D:78:GLU:HG2	2:P:301:PRO:HG3	1.86	0.58
1:F:114:VAL:HG23	1:F:122:MET:CE	2.33	0.58
1:B:131:PHE:CD2	1:B:138:HIS:HB3	2.38	0.58
2:M:360:ASP:OD2	2:M:428:ARG:HD2	2.03	0.58
1:A:163:GLN:HG3	1:C:61:HIS:ND1	2.19	0.58
1:C:100:ASP:OD1	1:C:100:ASP:N	2.36	0.57
2:O:390:LYS:HE2	6:O:727:HOH:O	2.04	0.57
2:Q:359:HIS:O	2:Q:366:ASN:HB3	2.04	0.57
2:Q:364:LEU:HD22	2:Q:440:ARG:HD3	1.86	0.57
2:M:390:LYS:HD3	6:M:639:HOH:O	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:416:LEU:C	2:O:416:LEU:HD23	2.24	0.57
2:P:497:ASN:ND2	2:P:499:GLU:HB2	2.19	0.57
2:R:364:LEU:HD22	2:R:440:ARG:HD3	1.85	0.57
2:N:462:HIS:HE1	5:N:550:3HP:H4	1.70	0.57
1:F:41:LYS:HD2	1:F:88:ALA:HA	1.85	0.57
1:F:67:PHE:HZ	1:F:94:ARG:HD2	1.69	0.57
1:C:41:LYS:HD2	1:C:88:ALA:HA	1.87	0.57
1:E:184:ARG:NH1	1:E:184:ARG:HG3	2.19	0.57
1:B:39:LEU:HD11	1:B:93:GLY:HA3	1.87	0.57
1:B:177:VAL:O	1:B:180:LYS:HB3	2.04	0.57
1:E:176:GLU:OE2	1:E:179:GLY:HA2	2.05	0.57
2:N:478:LEU:C	2:N:478:LEU:HD23	2.25	0.57
1:F:176:GLU:CG	1:F:179:GLY:HA2	2.33	0.57
1:D:19:ILE:HG22	1:D:26:ALA:HB1	1.86	0.56
2:R:497:ASN:ND2	2:R:499:GLU:HB2	2.21	0.56
2:O:356:PHE:CD1	2:O:428:ARG:HD3	2.40	0.56
2:O:390:LYS:HD3	6:O:645:HOH:O	2.05	0.56
2:P:390:LYS:HD3	6:P:649:HOH:O	2.04	0.56
1:E:100:ASP:CG	1:E:101:ALA:H	2.09	0.56
2:M:497:ASN:HD22	2:M:498:PRO:N	2.04	0.56
1:C:163:GLN:HB3	1:C:165:GLN:HE21	1.68	0.56
2:R:536:GLU:HB2	6:R:1362:HOH:O	2.05	0.56
2:M:478:LEU:HD23	2:M:478:LEU:C	2.27	0.56
1:C:27:GLY:HA3	2:O:411:LYS:HE3	1.89	0.55
1:F:25:ALA:O	2:R:411:LYS:HE3	2.07	0.55
1:B:176:GLU:HG3	1:B:180:LYS:C	2.26	0.55
2:O:364:LEU:HD22	2:O:440:ARG:CD	2.37	0.55
2:P:356:PHE:CD1	2:P:428:ARG:HD3	2.41	0.55
1:E:176:GLU:HG2	1:E:179:GLY:HA2	1.89	0.55
1:F:19:ILE:O	2:R:426:VAL:HG21	2.07	0.55
1:B:176:GLU:HA	1:B:180:LYS:O	2.06	0.55
1:C:177:VAL:O	1:C:180:LYS:HB3	2.07	0.55
2:P:383:ARG:NE	2:P:434:ASP:O	2.35	0.55
1:A:39:LEU:HD11	1:A:93:GLY:HA3	1.88	0.54
1:B:176:GLU:HG2	1:B:179:GLY:HA2	1.89	0.54
1:E:110:LYS:NZ	1:E:147:ASP:OD1	2.39	0.54
1:E:176:GLU:HA	1:E:180:LYS:O	2.08	0.54
2:Q:497:ASN:HD22	2:Q:498:PRO:N	2.05	0.54
2:M:497:ASN:ND2	2:M:499:GLU:HB2	2.23	0.54
2:P:364:LEU:HD11	2:P:442:ILE:HG23	1.89	0.54
1:F:115:ASN:HA	1:F:121:PRO:HA	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:497:ASN:HD22	2:M:497:ASN:C	2.11	0.53
1:A:176:GLU:HG2	1:A:179:GLY:HA2	1.91	0.53
2:N:497:ASN:HD21	2:N:499:GLU:HB2	1.73	0.53
1:A:35:ILE:HD13	2:M:351:PHE:CE1	2.43	0.53
1:B:163:GLN:HB3	1:B:165:GLN:HE22	1.74	0.53
2:O:400:TRP:HA	2:O:425:GLY:O	2.09	0.53
1:D:51:LEU:O	1:D:105:THR:HA	2.08	0.53
2:P:434:ASP:HB3	2:P:436:TYR:CE2	2.43	0.53
1:F:98:THR:O	1:F:102:GLY:HA2	2.08	0.53
1:D:50:LEU:O	1:D:182:ALA:HA	2.09	0.53
2:O:462:HIS:HE1	5:O:550:3HP:H4	1.73	0.53
1:D:153:ALA:HB3	1:D:154:LYS:HE3	1.90	0.53
2:P:376:GLU:O	2:P:442:ILE:HA	2.08	0.53
1:A:18:HIS:CE1	1:A:99:PHE:CE1	2.97	0.53
2:O:410:HIS:CE1	2:O:412:ASN:H	2.27	0.52
1:F:67:PHE:CZ	1:F:94:ARG:HD2	2.44	0.52
2:O:449:TRP:CE3	5:O:550:3HP:H71	2.45	0.52
1:E:131:PHE:CD2	1:E:138:HIS:HB3	2.45	0.52
1:F:78:GLU:HB3	1:F:80:GLN:NE2	2.24	0.52
2:O:361:HIS:CG	4:O:601:BME:H21	2.44	0.52
1:A:114:VAL:HG23	1:A:122:MET:CE	2.39	0.52
1:D:144:TYR:CE1	1:D:158:LEU:HD13	2.44	0.52
2:R:497:ASN:HD21	2:R:499:GLU:HB2	1.75	0.52
2:R:326:THR:HG22	2:R:330:ARG:HD2	1.92	0.52
1:E:50:LEU:HB2	1:E:180:LYS:HE3	1.91	0.52
1:F:78:GLU:HG2	2:R:301:PRO:CG	2.38	0.52
1:B:78:GLU:HG2	2:N:301:PRO:HG2	1.92	0.51
2:N:414:ARG:NE	2:N:414:ARG:HA	2.24	0.51
1:C:163:GLN:CB	1:C:165:GLN:HE22	2.24	0.51
2:M:497:ASN:ND2	2:M:499:GLU:N	2.50	0.51
2:O:410:HIS:ND1	2:O:412:ASN:N	2.52	0.51
2:Q:447:TYR:CE2	2:Q:460:HIS:CE1	2.98	0.51
1:C:44:ALA:O	1:C:48:HIS:NE2	2.30	0.51
1:D:143:LEU:C	1:D:143:LEU:HD23	2.31	0.51
2:P:410:HIS:CE1	2:P:412:ASN:H	2.28	0.51
1:A:65:ASP:OD2	1:A:133:ARG:HD3	2.10	0.51
2:O:434:ASP:HB3	2:O:436:TYR:CE2	2.46	0.51
1:D:163:GLN:HG3	1:F:61:HIS:ND1	2.25	0.51
2:N:376:GLU:O	2:N:442:ILE:HA	2.10	0.51
2:Q:505:ILE:O	2:Q:507:LYS:HE3	2.09	0.51
2:O:497:ASN:HD22	2:O:497:ASN:C	2.14	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:PHE:CD2	1:A:138:HIS:HB3	2.46	0.51
1:D:32:ASP:HB2	6:P:733:HOH:O	2.10	0.51
2:R:416:LEU:C	2:R:416:LEU:HD23	2.31	0.51
1:A:44:ALA:O	1:A:48:HIS:NE2	2.30	0.51
2:M:390:LYS:CD	6:M:639:HOH:O	2.59	0.51
1:B:190:GLN:HG3	2:N:333:ARG:HG2	1.92	0.50
1:C:131:PHE:O	1:C:132:ALA:HB2	2.11	0.50
2:M:497:ASN:HD21	2:M:499:GLU:HB2	1.77	0.50
1:C:176:GLU:HG3	1:C:180:LYS:O	2.12	0.50
2:O:359:HIS:O	2:O:366:ASN:HB3	2.11	0.50
1:A:176:GLU:HG2	1:A:179:GLY:CA	2.41	0.50
2:M:364:LEU:HD22	2:M:440:ARG:HD3	1.93	0.50
1:C:176:GLU:HG2	1:C:179:GLY:HA2	1.94	0.50
1:D:176:GLU:CG	1:D:179:GLY:HA2	2.41	0.50
1:E:19:ILE:HG22	1:E:26:ALA:HB1	1.94	0.50
2:M:356:PHE:CD1	2:M:428:ARG:HD3	2.47	0.50
2:R:536:GLU:HG3	6:R:1254:HOH:O	2.11	0.50
2:M:364:LEU:HD22	2:M:440:ARG:CD	2.42	0.50
2:O:360:ASP:HB3	2:O:428:ARG:HG3	1.94	0.50
1:E:176:GLU:HG3	1:E:180:LYS:O	2.11	0.50
2:P:359:HIS:O	2:P:366:ASN:HB3	2.11	0.49
1:C:50:LEU:O	1:C:182:ALA:HA	2.12	0.49
2:Q:315:TRP:HZ2	2:Q:503:GLN:NE2	2.09	0.49
2:M:462:HIS:CE1	5:M:550:3HP:H4	2.45	0.49
2:N:326:THR:HG22	2:N:330:ARG:HD2	1.93	0.49
2:O:381:ALA:O	2:O:522:ARG:HA	2.13	0.49
2:Q:405:GLY:HA3	6:Q:1044:HOH:O	2.12	0.49
2:O:505:ILE:O	2:O:507:LYS:HE3	2.13	0.49
1:A:61:HIS:ND1	1:B:163:GLN:HG3	2.28	0.49
1:A:176:GLU:HG3	1:A:180:LYS:N	2.27	0.49
2:P:313:ARG:O	2:P:318:LYS:CE	2.61	0.49
1:F:147:ASP:OD2	1:F:174:ARG:HD2	2.13	0.49
2:R:449:TRP:CE3	5:R:550:3HP:H71	2.48	0.49
2:M:356:PHE:HD1	2:M:428:ARG:HD3	1.77	0.49
1:D:163:GLN:HB3	1:D:165:GLN:HE22	1.77	0.49
2:O:356:PHE:HD1	2:O:428:ARG:CD	2.25	0.49
2:P:416:LEU:C	2:P:416:LEU:CD2	2.81	0.49
2:M:363:LEU:HD23	2:M:425:GLY:HA2	1.95	0.49
1:E:131:PHE:CE2	1:E:138:HIS:HB3	2.48	0.49
2:P:411:LYS:O	2:P:414:ARG:NH1	2.46	0.48
2:R:489:CYS:HA	2:R:490:PRO:HD3	1.70	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:434:ASP:HB3	2:N:436:TYR:CE2	2.47	0.48
1:D:64:ARG:HD3	1:D:99:PHE:O	2.13	0.48
1:D:176:GLU:HG3	1:D:180:LYS:N	2.28	0.48
1:D:191:GLY:O	1:D:194:GLU:HB2	2.12	0.48
1:F:31:ARG:NH1	2:R:428:ARG:HG2	2.29	0.48
1:C:98:THR:O	1:C:102:GLY:HA2	2.13	0.48
2:Q:364:LEU:HB2	2:Q:440:ARG:HD3	1.95	0.48
2:Q:416:LEU:HD23	2:Q:416:LEU:C	2.33	0.48
1:F:114:VAL:HG23	1:F:122:MET:HE2	1.95	0.48
2:O:361:HIS:CD2	6:O:706:HOH:O	2.66	0.48
2:O:497:ASN:ND2	2:O:499:GLU:HB2	2.28	0.48
1:E:188:ARG:HG3	1:E:188:ARG:HH11	1.79	0.48
2:Q:407:ARG:HG2	2:Q:407:ARG:HH11	1.78	0.48
1:E:98:THR:O	1:E:102:GLY:HA2	2.14	0.48
2:Q:484:PRO:O	2:Q:487:PRO:HD2	2.14	0.48
2:O:383:ARG:HG3	2:O:436:TYR:CE1	2.49	0.48
1:F:84:ASN:OD1	1:F:86:GLU:HB2	2.12	0.48
2:M:486:ILE:HB	2:M:487:PRO:HD3	1.96	0.48
2:Q:438:SER:O	4:Q:601:BME:H22	2.13	0.48
2:R:416:LEU:HD23	2:R:417:ALA:N	2.29	0.48
1:C:39:LEU:HD11	1:C:93:GLY:HA3	1.95	0.47
1:C:143:LEU:HD23	1:C:143:LEU:C	2.34	0.47
2:Q:447:TYR:CE2	2:Q:460:HIS:HE1	2.31	0.47
2:O:376:GLU:O	2:O:442:ILE:HA	2.13	0.47
2:O:473:LYS:HD2	2:O:474:LEU:N	2.30	0.47
1:E:168:GLU:CA	1:E:171:ILE:HD12	2.42	0.47
2:P:307:ARG:HG2	2:P:533:THR:HG22	1.97	0.47
1:E:53:GLY:O	1:E:103:GLU:HG3	2.14	0.47
2:Q:364:LEU:HD22	2:Q:440:ARG:CD	2.43	0.47
2:M:473:LYS:HD2	2:M:474:LEU:N	2.29	0.47
1:C:134:GLY:HA3	2:O:326:THR:HG22	1.95	0.47
2:R:392:VAL:HG12	2:R:395:THR:HB	1.95	0.47
1:E:8:THR:HA	1:E:9:PRO:HD3	1.77	0.47
2:Q:400:TRP:HA	2:Q:425:GLY:O	2.14	0.47
1:F:74:ASP:HB2	6:F:1293:HOH:O	2.14	0.47
2:Q:361:HIS:ND1	4:Q:601:BME:H21	2.30	0.47
2:Q:392:VAL:HG12	2:Q:395:THR:HB	1.97	0.47
2:O:356:PHE:CE1	2:O:428:ARG:HD3	2.50	0.47
1:F:41:LYS:O	1:F:48:HIS:HE1	1.98	0.47
1:F:64:ARG:HD3	1:F:99:PHE:O	2.15	0.47
1:B:35:ILE:HG21	1:B:92:PHE:HE2	1.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:PHE:CD2	2:M:475:ILE:HD12	2.50	0.46
1:A:180:LYS:HG2	1:A:181:THR:N	2.29	0.46
2:M:495:ILE:CG2	2:M:500:ALA:HB3	2.46	0.46
2:O:399:MET:HA	2:O:462:HIS:O	2.16	0.46
1:D:61:HIS:CD2	1:E:165:GLN:OE1	2.69	0.46
2:P:489:CYS:HA	2:P:490:PRO:HD3	1.77	0.46
1:E:176:GLU:HG2	1:E:179:GLY:CA	2.45	0.46
2:Q:307:ARG:HG2	2:Q:533:THR:HG22	1.97	0.46
2:Q:361:HIS:CD2	2:Q:361:HIS:N	2.72	0.46
2:R:307:ARG:HG2	2:R:533:THR:HG22	1.98	0.46
1:A:176:GLU:OE2	1:A:179:GLY:CA	2.55	0.46
1:F:168:GLU:HA	1:F:171:ILE:HD12	1.97	0.46
1:D:78:GLU:HG2	2:P:301:PRO:CG	2.45	0.46
2:R:478:LEU:C	2:R:478:LEU:HD23	2.36	0.46
1:A:165:GLN:NE2	1:C:61:HIS:NE2	2.64	0.46
2:N:400:TRP:HA	2:N:425:GLY:O	2.16	0.46
2:O:410:HIS:CE1	2:O:412:ASN:HB2	2.50	0.46
2:M:307:ARG:HG2	2:M:533:THR:HG22	1.98	0.46
1:D:134:GLY:HA3	2:P:326:THR:HG22	1.96	0.46
1:E:13:ALA:HB2	2:Q:475:ILE:HG21	1.97	0.46
2:R:413:ASP:C	2:R:414:ARG:HD2	2.35	0.46
2:R:491:ILE:CD1	5:R:550:3HP:H6	2.46	0.46
1:B:98:THR:O	1:B:102:GLY:HA2	2.16	0.46
1:D:36:TRP:CE3	1:D:36:TRP:HA	2.50	0.46
2:Q:326:THR:HG22	2:Q:330:ARG:HD2	1.98	0.46
1:B:50:LEU:O	1:B:182:ALA:HA	2.16	0.46
1:B:114:VAL:HG22	6:B:319:HOH:O	2.16	0.46
2:P:478:LEU:C	2:P:478:LEU:HD23	2.36	0.46
2:Q:451:ASN:HB3	2:Q:455:ASP:OD2	2.16	0.46
2:M:385:VAL:O	2:M:526:VAL:HA	2.17	0.45
1:B:100:ASP:CG	1:B:101:ALA:H	2.19	0.45
2:M:359:HIS:O	2:M:366:ASN:HB3	2.16	0.45
1:B:132:ALA:HB3	1:B:135:ILE:HD12	1.98	0.45
2:Q:399:MET:HA	2:Q:462:HIS:O	2.16	0.45
2:M:522:ARG:HH11	2:M:522:ARG:HD3	1.49	0.45
1:E:123:ALA:HB3	1:E:144:TYR:CE2	2.51	0.45
2:Q:390:LYS:HA	2:Q:391:PRO:HD3	1.85	0.45
2:M:489:CYS:HA	2:M:490:PRO:HD3	1.79	0.45
2:M:495:ILE:HG21	2:M:500:ALA:HB3	1.98	0.45
1:D:31:ARG:NH2	6:D:932:HOH:O	2.35	0.45
2:P:362:ASP:OD1	2:P:440:ARG:HD2	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:70:VAL:HG12	1:E:128:ILE:HG12	1.99	0.45
1:E:98:THR:HG1	1:E:101:ALA:HB3	1.81	0.45
1:C:165:GLN:H	1:C:165:GLN:HE21	1.64	0.45
2:Q:408:TYR:HE1	2:Q:447:TYR:CZ	2.34	0.45
1:F:125:HIS:HA	1:F:143:LEU:O	2.16	0.45
1:A:24:GLU:HB2	6:A:262:HOH:O	2.17	0.45
2:Q:420:ASP:HA	2:Q:421:PRO:HD2	1.78	0.45
1:F:100:ASP:OD1	1:F:100:ASP:N	2.32	0.45
1:F:100:ASP:CG	1:F:101:ALA:N	2.66	0.45
2:P:400:TRP:HA	2:P:425:GLY:O	2.16	0.45
1:E:41:LYS:CD	1:E:88:ALA:HA	2.30	0.45
2:Q:489:CYS:HA	2:Q:490:PRO:HD3	1.82	0.45
1:B:36:TRP:HA	1:B:36:TRP:CE3	2.52	0.45
2:N:392:VAL:HG12	2:N:395:THR:HB	1.98	0.45
1:D:35:ILE:HG21	1:D:92:PHE:HE2	1.82	0.45
1:E:61:HIS:ND1	1:F:163:GLN:HG3	2.31	0.45
1:F:48:HIS:HA	1:F:109:VAL:HG12	1.98	0.45
2:M:497:ASN:HD22	2:M:499:GLU:N	2.00	0.45
1:B:19:ILE:HD11	2:N:408:TYR:HD1	1.82	0.45
2:P:497:ASN:HA	2:P:498:PRO:HD2	1.74	0.45
2:N:362:ASP:OD1	2:N:440:ARG:HD3	2.17	0.44
2:R:359:HIS:O	2:R:366:ASN:HB3	2.17	0.44
1:E:50:LEU:O	1:E:182:ALA:HA	2.18	0.44
2:M:354:LEU:HD23	2:M:356:PHE:CE1	2.52	0.44
2:M:448:PRO:HB2	2:P:516:MET:HA	1.99	0.44
1:F:174:ARG:HE	1:F:181:THR:HG23	1.81	0.44
2:M:307:ARG:NE	2:M:536:GLU:OE2	2.51	0.44
1:C:48:HIS:HA	1:C:109:VAL:HG12	2.00	0.44
1:B:140:HIS:O	1:B:197:PHE:HA	2.17	0.44
1:E:51:LEU:HB2	1:E:106:LEU:HB3	1.98	0.44
2:N:489:CYS:HA	2:N:490:PRO:HD3	1.87	0.44
1:F:8:THR:HA	1:F:9:PRO:HD3	1.87	0.44
2:M:360:ASP:HB3	2:M:428:ARG:HG3	1.99	0.44
1:B:61:HIS:ND1	1:C:163:GLN:HG3	2.32	0.44
2:P:360:ASP:HB3	2:P:428:ARG:HG3	1.99	0.44
2:O:410:HIS:ND1	2:O:411:LYS:N	2.66	0.43
2:P:462:HIS:CE1	5:P:550:3HP:H4	2.45	0.43
1:E:44:ALA:O	1:E:48:HIS:NE2	2.32	0.43
1:E:114:VAL:HG23	1:E:122:MET:CE	2.48	0.43
1:A:19:ILE:HG22	1:A:26:ALA:HB1	1.99	0.43
1:A:19:ILE:HG21	2:M:410:HIS:HB2	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:GLU:HG2	2:M:301:PRO:CB	2.48	0.43
2:Q:362:ASP:OD1	2:Q:440:ARG:HD2	2.18	0.43
1:B:131:PHE:CE2	1:B:138:HIS:HB3	2.52	0.43
1:D:48:HIS:HA	1:D:109:VAL:HG12	1.99	0.43
2:P:315:TRP:HZ2	2:P:503:GLN:HE21	1.66	0.43
1:E:165:GLN:H	1:E:165:GLN:HE21	0.62	0.43
1:F:114:VAL:HG23	1:F:122:MET:HE3	2.00	0.43
1:A:132:ALA:HB3	1:A:135:ILE:HD12	1.98	0.43
2:P:318:LYS:HD3	2:P:318:LYS:HA	1.72	0.43
2:Q:497:ASN:ND2	2:Q:499:GLU:N	2.62	0.43
1:C:54:GLN:HG3	1:C:184:ARG:HH22	1.83	0.43
1:D:52:LEU:C	1:D:52:LEU:HD22	2.38	0.43
2:P:307:ARG:CG	2:P:533:THR:HG22	2.48	0.43
2:P:486:ILE:HB	2:P:487:PRO:HD3	2.00	0.43
1:E:177:VAL:O	1:E:180:LYS:HB3	2.18	0.43
2:R:399:MET:HA	2:R:462:HIS:O	2.19	0.43
1:C:51:LEU:HD12	1:C:106:LEU:HD23	2.01	0.43
1:C:65:ASP:OD2	1:C:133:ARG:HD3	2.18	0.43
2:P:437:TYR:CD1	2:P:437:TYR:C	2.92	0.43
1:E:18:HIS:CE1	1:E:99:PHE:HE1	2.37	0.43
1:F:143:LEU:C	1:F:143:LEU:HD23	2.39	0.43
2:M:505:ILE:O	2:M:507:LYS:HE3	2.19	0.43
2:O:318:LYS:HD3	2:O:318:LYS:HA	1.88	0.43
1:D:28:ASN:HB3	1:D:29:PRO:HD2	2.01	0.43
1:F:98:THR:HG1	1:F:101:ALA:HB3	1.83	0.43
2:P:447:TYR:HA	2:P:448:PRO:HD3	1.88	0.43
1:F:163:GLN:HA	1:F:164:PRO:HD2	1.78	0.43
2:R:447:TYR:HB2	2:R:448:PRO:HD2	2.00	0.43
2:R:497:ASN:HA	2:R:498:PRO:HD3	1.83	0.43
2:O:362:ASP:OD1	2:O:364:LEU:HB2	2.19	0.43
1:F:177:VAL:HG12	1:F:178:ASP:OD2	2.19	0.43
2:M:310:ILE:HG13	2:O:453:PRO:HB2	2.00	0.43
2:M:400:TRP:HA	2:M:425:GLY:O	2.18	0.43
1:C:3:GLU:OE1	1:C:3:GLU:HA	2.18	0.43
2:O:489:CYS:HA	2:O:490:PRO:HD3	1.74	0.43
2:R:486:ILE:HB	2:R:487:PRO:HD3	2.01	0.43
1:A:54:GLN:HG2	1:A:102:GLY:O	2.18	0.42
2:M:315:TRP:HZ2	2:M:503:GLN:NE2	2.16	0.42
1:B:120:VAL:HA	1:B:121:PRO:HD3	1.86	0.42
1:F:19:ILE:HD13	1:F:19:ILE:HG21	1.75	0.42
2:R:383:ARG:HD2	2:R:436:TYR:CZ	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:PHE:CD2	1:C:138:HIS:HB3	2.54	0.42
1:D:52:LEU:HA	1:D:104:TRP:O	2.19	0.42
2:Q:362:ASP:OD1	2:Q:440:ARG:CD	2.66	0.42
2:Q:495:ILE:CG2	2:Q:500:ALA:HB3	2.49	0.42
2:P:302:ALA:HB1	2:P:347:THR:CG2	2.49	0.42
1:F:78:GLU:HB3	1:F:80:GLN:HE21	1.84	0.42
2:N:497:ASN:HD22	2:N:499:GLU:N	2.10	0.42
2:P:414:ARG:NE	2:P:414:ARG:HA	2.34	0.42
2:R:405:GLY:HA3	6:R:1285:HOH:O	2.20	0.42
2:N:361:HIS:CG	4:N:601:BME:H21	2.55	0.42
2:R:505:ILE:HG22	2:R:507:LYS:CE	2.37	0.42
2:O:361:HIS:HD2	6:O:706:HOH:O	2.02	0.42
1:A:19:ILE:CG2	2:M:410:HIS:HB2	2.49	0.42
1:B:123:ALA:HB3	1:B:144:TYR:CE2	2.54	0.42
1:C:18:HIS:HA	1:C:22:ALA:HB3	2.02	0.42
2:O:304:ASP:HB2	2:O:343:ILE:HB	2.02	0.42
1:A:78:GLU:HG2	2:M:301:PRO:HG3	2.02	0.42
1:A:100:ASP:OD1	1:A:100:ASP:N	2.44	0.42
1:C:52:LEU:CD2	1:C:184:ARG:NH1	2.82	0.42
1:A:25:ALA:C	1:A:27:GLY:H	2.23	0.42
1:A:114:VAL:HG23	1:A:122:MET:HE3	2.01	0.42
2:O:361:HIS:H	2:O:361:HIS:HD2	1.62	0.42
1:D:98:THR:OG1	1:D:101:ALA:HB3	2.20	0.42
1:E:51:LEU:HD11	1:E:126:ILE:HD12	2.02	0.42
1:E:52:LEU:HA	1:E:104:TRP:O	2.20	0.42
2:R:415:TYR:CE1	2:R:416:LEU:HD22	2.54	0.42
5:M:550:3HP:C6	6:M:741:HOH:O	2.68	0.41
1:C:184:ARG:NH1	1:C:184:ARG:HG3	2.35	0.41
1:D:15:PRO:HB3	1:D:133:ARG:HD3	2.01	0.41
1:F:17:VAL:CG2	1:F:21:LEU:HD12	2.49	0.41
2:R:497:ASN:HD21	2:R:499:GLU:CB	2.33	0.41
1:B:20:GLY:HA2	2:N:426:VAL:HG13	2.02	0.41
1:C:161:ILE:HD13	1:C:196:VAL:HG21	2.01	0.41
2:O:497:ASN:HD21	2:O:499:GLU:HB2	1.85	0.41
1:D:100:ASP:OD1	1:D:100:ASP:N	2.40	0.41
1:E:98:THR:OG1	1:E:101:ALA:HB3	2.20	0.41
2:Q:407:ARG:HG2	2:Q:407:ARG:NH1	2.35	0.41
1:F:147:ASP:OD2	1:F:174:ARG:NH1	2.53	0.41
2:R:362:ASP:OD1	2:R:440:ARG:HD2	2.20	0.41
2:R:385:VAL:O	2:R:526:VAL:HA	2.19	0.41
1:A:100:ASP:CG	1:A:101:ALA:N	2.70	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:GLU:HG3	1:A:180:LYS:C	2.40	0.41
2:R:390:LYS:HA	2:R:391:PRO:HD3	1.86	0.41
1:D:153:ALA:CB	1:D:154:LYS:HE3	2.50	0.41
2:Q:478:LEU:C	2:Q:478:LEU:HD23	2.41	0.41
2:N:372:LEU:HA	2:N:373:PRO:HD3	1.93	0.41
2:O:497:ASN:HD22	2:O:498:PRO:N	2.18	0.41
2:Q:447:TYR:CZ	2:Q:460:HIS:HE1	2.39	0.41
2:R:497:ASN:ND2	2:R:497:ASN:C	2.72	0.41
2:M:416:LEU:C	2:M:416:LEU:HD23	2.41	0.41
2:P:410:HIS:ND1	2:P:411:LYS:N	2.68	0.41
1:E:20:GLY:HA2	2:Q:426:VAL:HG13	2.02	0.41
1:E:35:ILE:HG21	1:E:92:PHE:HE2	1.85	0.41
1:B:98:THR:OG1	1:B:102:GLY:N	2.53	0.41
1:D:120:VAL:HA	1:D:121:PRO:HD3	1.89	0.41
2:Q:372:LEU:HA	2:Q:373:PRO:HD3	1.94	0.41
2:M:497:ASN:HA	2:M:498:PRO:HD2	1.81	0.41
1:B:70:VAL:HG21	1:B:106:LEU:HD21	2.02	0.41
1:B:124:PRO:HA	6:B:287:HOH:O	2.20	0.41
1:B:165:GLN:H	1:B:165:GLN:CD	2.07	0.41
1:C:52:LEU:C	1:C:52:LEU:HD22	2.41	0.41
1:C:100:ASP:CG	1:C:101:ALA:N	2.71	0.41
1:D:70:VAL:HG21	1:D:106:LEU:HD21	2.02	0.41
2:P:434:ASP:HB3	2:P:436:TYR:CD2	2.55	0.41
2:Q:462:HIS:CE1	5:Q:550:3HP:H4	2.50	0.41
2:R:364:LEU:HB2	2:R:440:ARG:HD3	2.02	0.41
1:A:4:LEU:HB3	2:M:387:GLN:HB3	2.02	0.41
1:B:143:LEU:HD23	1:B:143:LEU:C	2.41	0.41
2:Q:447:TYR:OH	2:Q:460:HIS:CE1	2.73	0.41
1:F:50:LEU:O	1:F:182:ALA:HA	2.20	0.41
2:R:361:HIS:CG	4:R:601:BME:H21	2.56	0.41
2:R:522:ARG:HH11	2:R:522:ARG:HD3	1.57	0.41
2:N:373:PRO:HB3	2:N:423:PHE:HB2	2.03	0.41
2:N:399:MET:HA	2:N:462:HIS:O	2.21	0.41
2:N:497:ASN:HD22	2:N:497:ASN:C	2.23	0.41
1:E:18:HIS:CE1	1:E:99:PHE:CE1	3.09	0.41
2:M:376:GLU:HG2	2:P:446:PRO:HD2	2.02	0.40
1:A:50:LEU:O	1:A:182:ALA:HA	2.21	0.40
2:N:364:LEU:HD22	2:N:440:ARG:HG2	2.03	0.40
2:N:489:CYS:HB3	2:N:492:VAL:HB	2.03	0.40
1:C:114:VAL:HG23	1:C:122:MET:CE	2.50	0.40
1:E:39:LEU:CD1	1:E:106:LEU:HD11	2.52	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:177:VAL:N	1:F:180:LYS:O	2.46	0.40
1:A:85:LEU:HD23	1:A:85:LEU:HA	1.91	0.40
1:B:92:PHE:CD1	2:N:349:PRO:HG3	2.56	0.40
2:P:392:VAL:HG12	2:P:395:THR:HB	2.03	0.40
2:P:497:ASN:HD21	2:P:499:GLU:HB2	1.86	0.40
1:C:52:LEU:HA	1:C:104:TRP:O	2.21	0.40
2:O:356:PHE:HD1	2:O:428:ARG:HD2	1.85	0.40
2:N:534:HIS:CE1	2:P:512:ASN:O	2.75	0.40
1:F:48:HIS:CD2	1:F:109:VAL:HG12	2.56	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	198/200 (99%)	193 (98%)	5 (2%)	0	100	100
1	B	198/200 (99%)	190 (96%)	8 (4%)	0	100	100
1	C	198/200 (99%)	192 (97%)	6 (3%)	0	100	100
1	D	198/200 (99%)	190 (96%)	8 (4%)	0	100	100
1	E	198/200 (99%)	187 (94%)	11 (6%)	0	100	100
1	F	198/200 (99%)	191 (96%)	7 (4%)	0	100	100
2	M	229/238 (96%)	220 (96%)	9 (4%)	0	100	100
2	N	229/238 (96%)	222 (97%)	7 (3%)	0	100	100
2	O	229/238 (96%)	222 (97%)	7 (3%)	0	100	100
2	P	229/238 (96%)	223 (97%)	6 (3%)	0	100	100
2	Q	229/238 (96%)	220 (96%)	9 (4%)	0	100	100
2	R	229/238 (96%)	218 (95%)	11 (5%)	0	100	100
All	All	2562/2628 (98%)	2468 (96%)	94 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	162/163 (99%)	154 (95%)	8 (5%)	25	17
1	B	162/163 (99%)	154 (95%)	8 (5%)	25	17
1	C	162/163 (99%)	156 (96%)	6 (4%)	34	27
1	D	162/163 (99%)	156 (96%)	6 (4%)	34	27
1	E	162/163 (99%)	156 (96%)	6 (4%)	34	27
1	F	162/163 (99%)	157 (97%)	5 (3%)	40	34
2	M	196/202 (97%)	185 (94%)	11 (6%)	21	13
2	N	196/202 (97%)	185 (94%)	11 (6%)	21	13
2	O	196/202 (97%)	187 (95%)	9 (5%)	27	19
2	P	196/202 (97%)	186 (95%)	10 (5%)	24	15
2	Q	196/202 (97%)	185 (94%)	11 (6%)	21	13
2	R	196/202 (97%)	189 (96%)	7 (4%)	35	28
All	All	2148/2190 (98%)	2050 (95%)	98 (5%)	27	19

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	19	ILE
1	A	38	ARG
1	A	52	LEU
1	A	106	LEU
1	A	133	ARG
1	A	145	PHE
1	A	165	GLN
2	M	301	PRO
2	M	372	LEU
2	M	395	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	M	416	LEU
2	M	428	ARG
2	M	434	ASP
2	M	473	LYS
2	M	478	LEU
2	M	497	ASN
2	M	507	LYS
2	M	534	HIS
1	B	4	LEU
1	B	32	ASP
1	B	52	LEU
1	B	106	LEU
1	B	133	ARG
1	B	141	THR
1	B	165	GLN
1	B	176	GLU
2	N	344	SER
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	442	ILE
2	N	497	ASN
2	N	507	LYS
2	N	534	HIS
1	C	4	LEU
1	C	19	ILE
1	C	38	ARG
1	C	52	LEU
1	C	150	GLN
1	C	165	GLN
2	O	372	LEU
2	O	393	PRO
2	O	395	THR
2	O	416	LEU
2	O	428	ARG
2	O	434	ASP
2	O	497	ASN
2	O	507	LYS
2	O	534	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	4	LEU
1	D	19	ILE
1	D	52	LEU
1	D	154	LYS
1	D	165	GLN
1	D	180	LYS
2	P	364	LEU
2	P	372	LEU
2	P	395	THR
2	P	414	ARG
2	P	416	LEU
2	P	434	ASP
2	P	478	LEU
2	P	497	ASN
2	P	503	GLN
2	P	534	HIS
1	E	4	LEU
1	E	38	ARG
1	E	52	LEU
1	E	150	GLN
1	E	165	GLN
1	E	180	LYS
2	Q	364	LEU
2	Q	372	LEU
2	Q	395	THR
2	Q	399	MET
2	Q	416	LEU
2	Q	428	ARG
2	Q	434	ASP
2	Q	442	ILE
2	Q	497	ASN
2	Q	507	LYS
2	Q	534	HIS
1	F	4	LEU
1	F	19	ILE
1	F	49	ILE
1	F	52	LEU
1	F	165	GLN
2	R	372	LEU
2	R	395	THR
2	R	416	LEU
2	R	428	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	R	434	ASP
2	R	440	ARG
2	R	497	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	GLN
2	M	361	HIS
2	M	412	ASN
2	M	497	ASN
2	M	503	GLN
1	B	80	GLN
1	B	165	GLN
2	N	361	HIS
2	N	412	ASN
2	N	497	ASN
2	N	503	GLN
1	C	165	GLN
2	O	361	HIS
2	O	412	ASN
2	O	497	ASN
2	O	503	GLN
1	D	165	GLN
2	P	361	HIS
2	P	412	ASN
2	P	497	ASN
2	P	503	GLN
1	E	165	GLN
2	Q	361	HIS
2	Q	412	ASN
2	Q	497	ASN
2	Q	503	GLN
1	F	165	GLN
2	R	361	HIS
2	R	497	ASN
2	R	503	GLN

5.3.3 RNA

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 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 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
4	BME	R	601	2	3,3,3	0.39	0	1,2,2	0.09	0
5	3HP	P	550	3	11,11,11	1.18	1 (9%)	14,14,14	1.54	4 (28%)
5	3HP	N	550	3	11,11,11	1.12	1 (9%)	14,14,14	2.18	5 (35%)
4	BME	N	601	2	3,3,3	0.15	0	1,2,2	0.57	0
4	BME	O	601	2	3,3,3	0.48	0	1,2,2	0.62	0
5	3HP	Q	550	3	11,11,11	1.20	0	14,14,14	1.82	5 (35%)
4	BME	Q	601	2	3,3,3	0.87	0	1,2,2	1.18	0
4	BME	M	601	2	3,3,3	0.38	0	1,2,2	0.10	0
5	3HP	O	550	3	11,11,11	1.05	0	14,14,14	1.67	6 (42%)
5	3HP	R	550	3	11,11,11	0.99	0	14,14,14	1.95	4 (28%)
5	3HP	M	550	3	11,11,11	1.23	1 (9%)	14,14,14	1.95	5 (35%)
4	BME	P	601	2	3,3,3	0.60	0	1,2,2	1.05	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
4	BME	R	601	2	-	0/1/1/1	-
5	3HP	P	550	3	-	0/4/4/4	0/1/1/1

Continued on next page...

Continued from previous page...

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	P	550	3HP	O1-C8	2.43	1.30	1.22
5	N	550	3HP	C2-C3	2.10	1.42	1.39
5	M	550	3HP	O1-C8	2.02	1.28	1.22

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	N	550	3HP	C7-C1-C6	-4.61	114.29	120.89
5	R	550	3HP	C7-C1-C6	-4.56	114.37	120.89
5	M	550	3HP	C7-C1-C6	-3.89	115.33	120.89
5	M	550	3HP	O1-C8-C7	-3.81	112.17	123.04
5	R	550	3HP	C7-C1-C2	3.66	126.18	120.38
5	Q	550	3HP	C7-C1-C6	-3.63	115.69	120.89
5	N	550	3HP	O1-C8-C7	-3.59	112.79	123.04
5	N	550	3HP	C7-C1-C2	3.51	125.94	120.38
5	M	550	3HP	C7-C1-C2	3.28	125.57	120.38
5	Q	550	3HP	C7-C1-C2	3.27	125.55	120.38
5	P	550	3HP	C7-C1-C6	-2.98	116.62	120.89
5	O	550	3HP	O1-C8-C7	-2.98	114.53	123.04
5	O	550	3HP	C7-C1-C6	-2.91	116.72	120.89
5	R	550	3HP	O1-C8-C7	-2.90	114.77	123.04
5	P	550	3HP	O1-C8-C7	-2.89	114.78	123.04
5	P	550	3HP	C7-C1-C2	2.66	124.59	120.38
5	Q	550	3HP	O1-C8-C7	-2.52	115.84	123.04
5	N	550	3HP	C3-C2-C1	-2.40	118.58	120.35
5	Q	550	3HP	C4-C3-C2	2.32	122.72	120.17
5	O	550	3HP	C4-C3-C2	2.28	122.67	120.17
5	O	550	3HP	O2-C8-C7	2.25	122.53	114.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	R	550	3HP	C3-C2-C1	-2.24	118.69	120.35
5	Q	550	3HP	C3-C2-C1	-2.17	118.75	120.35
5	N	550	3HP	O2-C8-C7	2.16	122.19	114.02
5	M	550	3HP	C3-C2-C1	-2.13	118.78	120.35
5	P	550	3HP	O2-C8-C7	2.10	121.99	114.02
5	O	550	3HP	C3-C2-C1	-2.06	118.83	120.35
5	M	550	3HP	O2-C8-C7	2.03	121.72	114.02
5	O	550	3HP	C7-C1-C2	2.01	123.56	120.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	R	601	BME	1	0
5	P	550	3HP	3	0
5	N	550	3HP	3	0
4	N	601	BME	1	0
4	O	601	BME	1	0
5	Q	550	3HP	3	0
4	Q	601	BME	3	0
5	O	550	3HP	3	0
5	R	550	3HP	4	0
5	M	550	3HP	4	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.