Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 11:48 PM GMT

PDB ID	:	1YKL
Title	:	Protocatechuate 3,4-Dioxygenase Y408C mutant bound to DHB
Authors	:	Brown, C.K.; Ohlendorf, D.H.
Deposited on	:	2005-01-18
Resolution	:	2.25 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

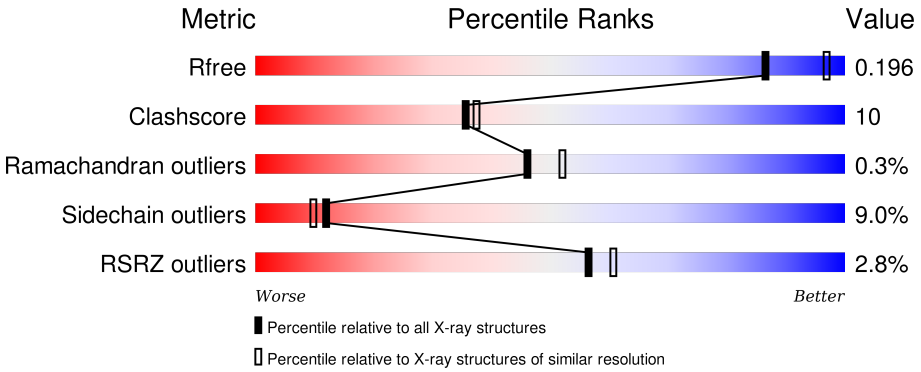
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1640 (2.28-2.24)
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (2.28-2.24)

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

Mol	Chain	Length	Quality of chain
1	A	200	2% 58% 33% 9% •
1	C	200	2% 51% 37% 11% •
1	E	200	2% 49% 38% 12% •
1	G	200	4% 57% 33% 8% •
1	I	200	5% 53% 35% 11% •

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Mol	Chain	Length	Quality of chain
1	K	200	6% 47% 38% 14%
2	B	238	3% 47% 38% 11% 5%
2	D	238	3% 48% 37% 13%
2	F	238	3% 58% 29% 10%
2	H	238	% 50% 38% 9%
2	J	238	3% 46% 39% 11% 5%
2	L	238	3% 50% 35% 12%

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
4	DHB	B	550	-	-	-	X
4	DHB	D	1550	-	-	-	X
4	DHB	F	2550	-	-	X	X
4	DHB	H	3550	-	-	-	X
4	DHB	J	4550	-	-	-	X
4	DHB	L	5550	-	-	X	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 21744 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 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	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	E	200	Total	C	N	O	S	0	0	0
			1571	993	276	299	3			
1	G	200	Total	C	N	O	S	0	0	0
			1571	993	276	299	3			
1	I	200	Total	C	N	O	S	0	0	0
			1571	993	276	299	3			
1	K	200	Total	C	N	O	S	0	0	0
			1571	993	276	299	3			

- Molecule 2 is a protein called Protocatechuate 3,4-dioxygenase beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	238	Total	C	N	O	S	0	1	0
			1875	1185	343	337	10			
2	D	238	Total	C	N	O	S	0	1	0
			1875	1185	343	337	10			
2	F	238	Total	C	N	O	S	0	1	0
			1875	1185	343	337	10			
2	H	238	Total	C	N	O	S	0	1	0
			1875	1185	343	337	10			
2	J	238	Total	C	N	O	S	0	1	0
			1875	1185	343	337	10			
2	L	238	Total	C	N	O	S	0	1	0
			1875	1185	343	337	10			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	408	CYS	TYR	ENGINEERED	UNP P00437

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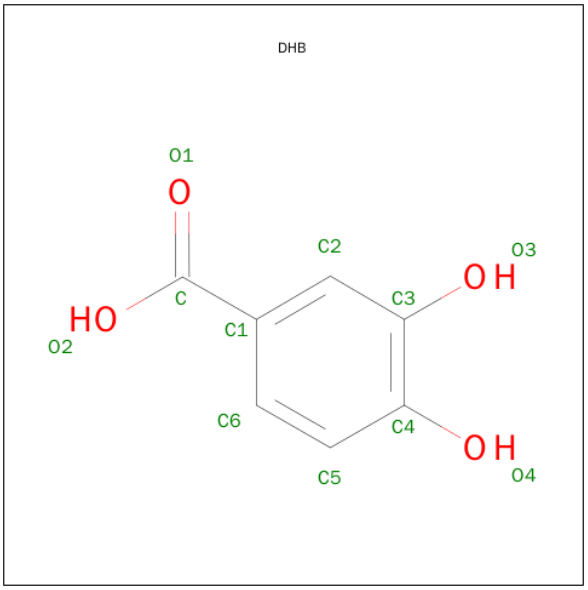
Chain	Residue	Modelled	Actual	Comment	Reference
D	408	CYS	TYR	ENGINEERED	UNP P00437
F	408	CYS	TYR	ENGINEERED	UNP P00437
H	408	CYS	TYR	ENGINEERED	UNP P00437
J	408	CYS	TYR	ENGINEERED	UNP P00437
L	408	CYS	TYR	ENGINEERED	UNP P00437

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	J	1	Total Fe 1 1	0	0
3	D	1	Total Fe 1 1	0	0
3	H	1	Total Fe 1 1	0	0
3	B	1	Total Fe 1 1	0	0
3	L	1	Total Fe 1 1	0	0
3	F	1	Total Fe 1 1	0	0

- Molecule 4 is 3,4-DIHYDROXYBENZOIC ACID (three-letter code: DHB) (formula: $C_7H_6O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 11 7 4	0	0
4	D	1	Total C O 11 7 4	0	0
4	F	1	Total C O 11 7 4	0	0
4	H	1	Total C O 11 7 4	0	0
4	J	1	Total C O 11 7 4	0	0
4	L	1	Total C O 11 7 4	0	0

- Molecule 5 is water.

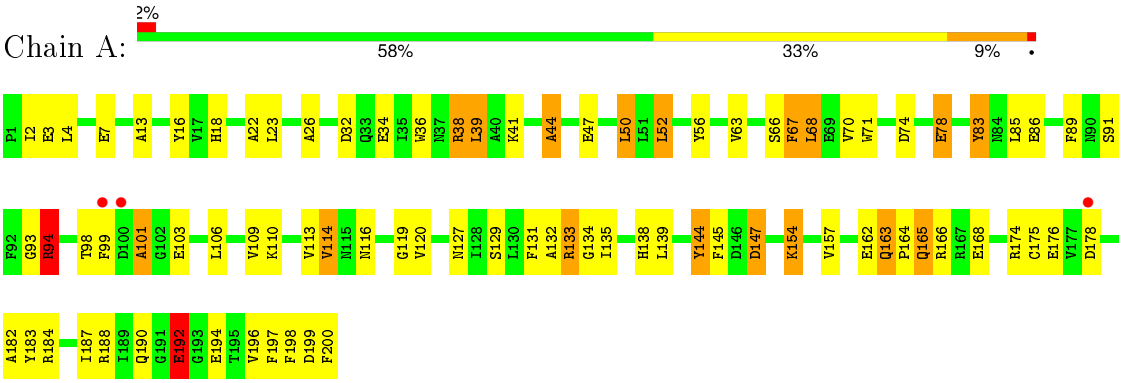
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	51	Total O 51 51	0	0
5	B	111	Total O 111 111	0	0
5	C	49	Total O 49 49	0	0
5	D	122	Total O 122 122	0	0
5	E	54	Total O 54 54	0	0
5	F	113	Total O 113 113	0	0
5	G	52	Total O 52 52	0	0
5	H	108	Total O 108 108	0	0
5	I	55	Total O 55 55	0	0
5	J	115	Total O 115 115	0	0
5	K	48	Total O 48 48	0	0
5	L	118	Total O 118 118	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 errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

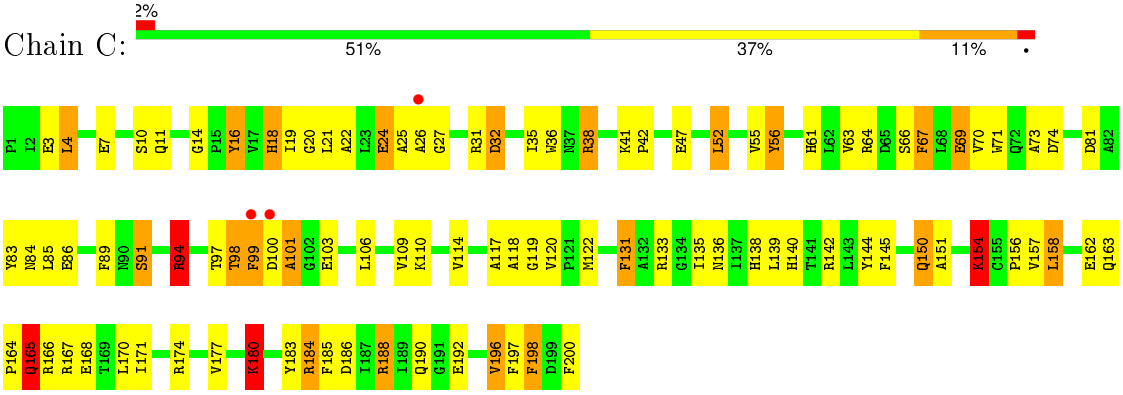
- Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain

Chain A:



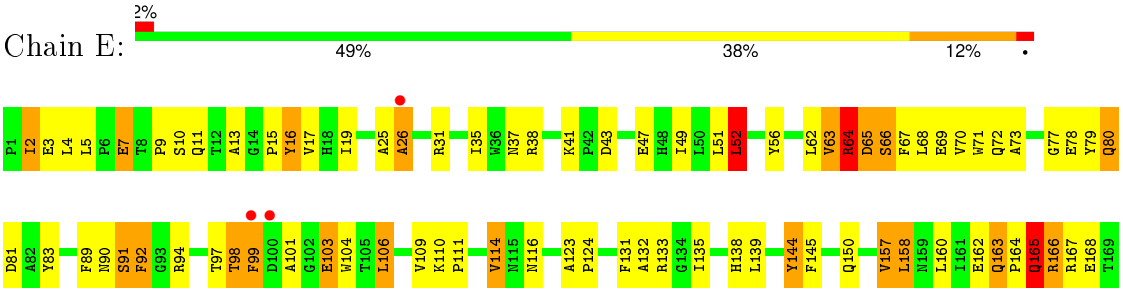
- Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain

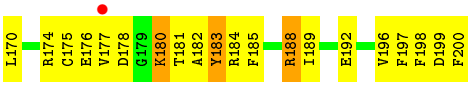
Chain C:



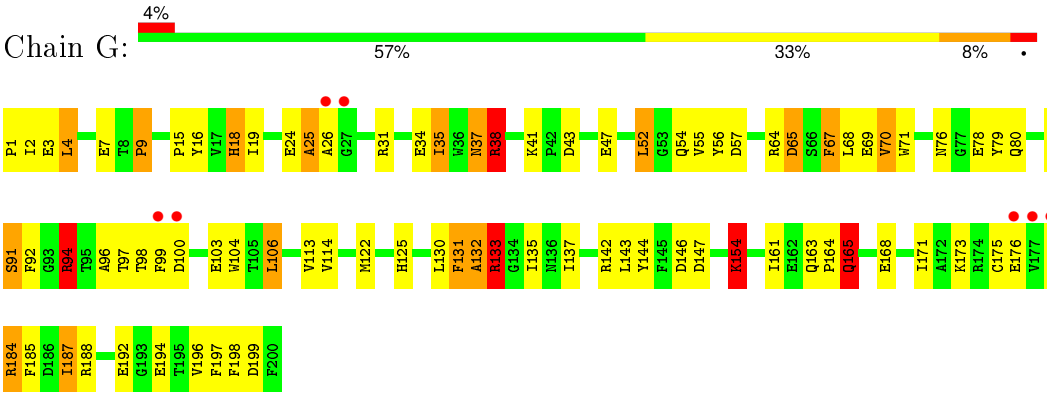
- Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain

Chain E:

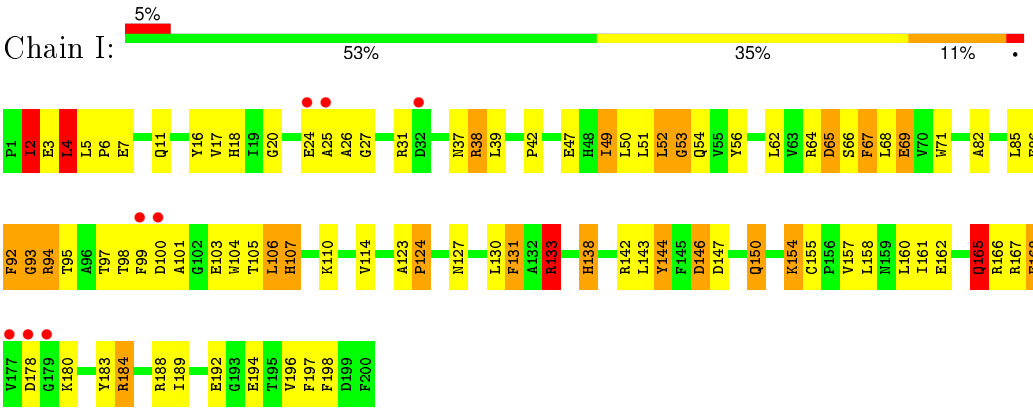




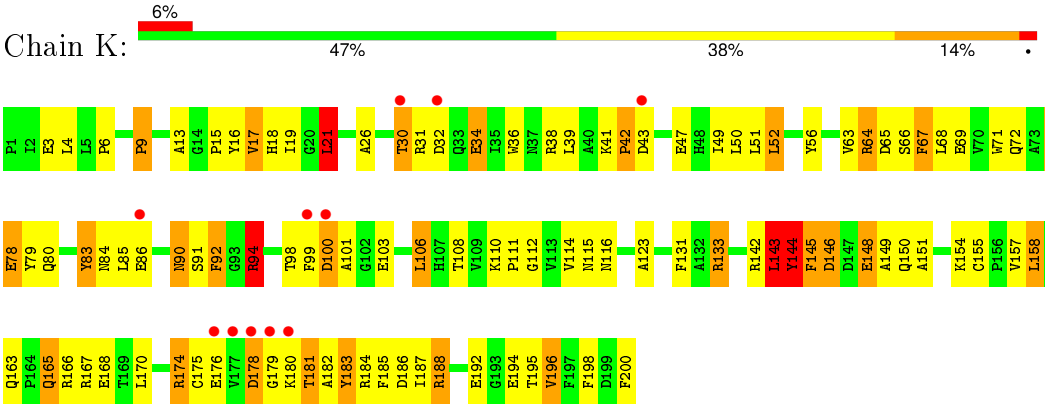
• Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain



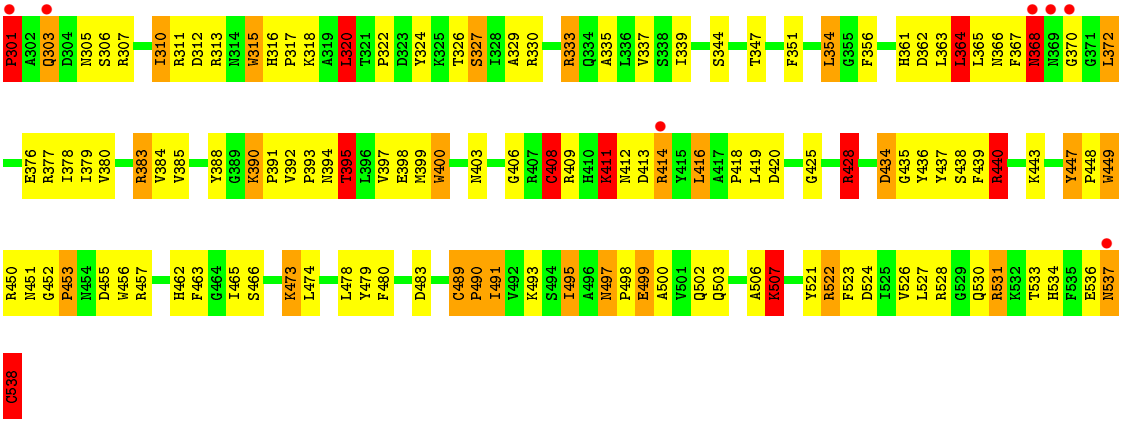
• Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain



• Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain

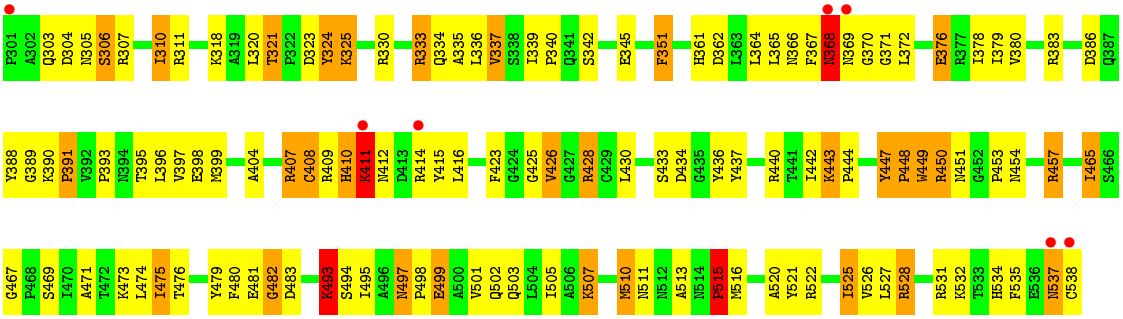


• Molecule 2: Protocatechuate 3,4-dioxygenase beta chain



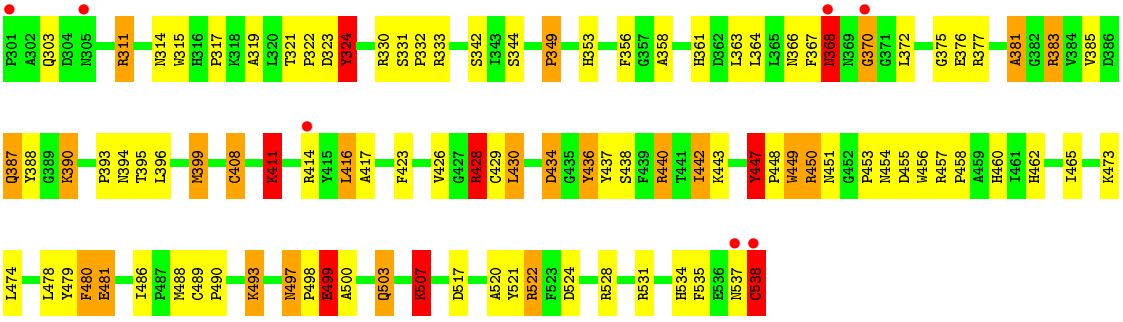
• Molecule 2: Protocatechuate 3,4-dioxygenase beta chain

Chain D:



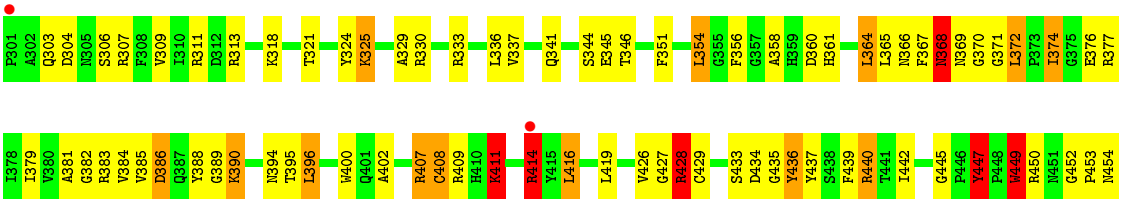
• Molecule 2: Protocatechuate 3,4-dioxygenase beta chain

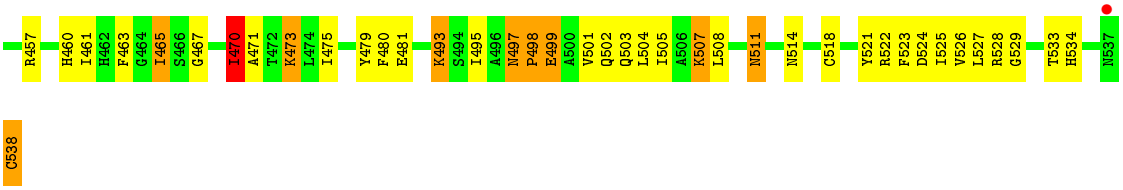
Chain F:



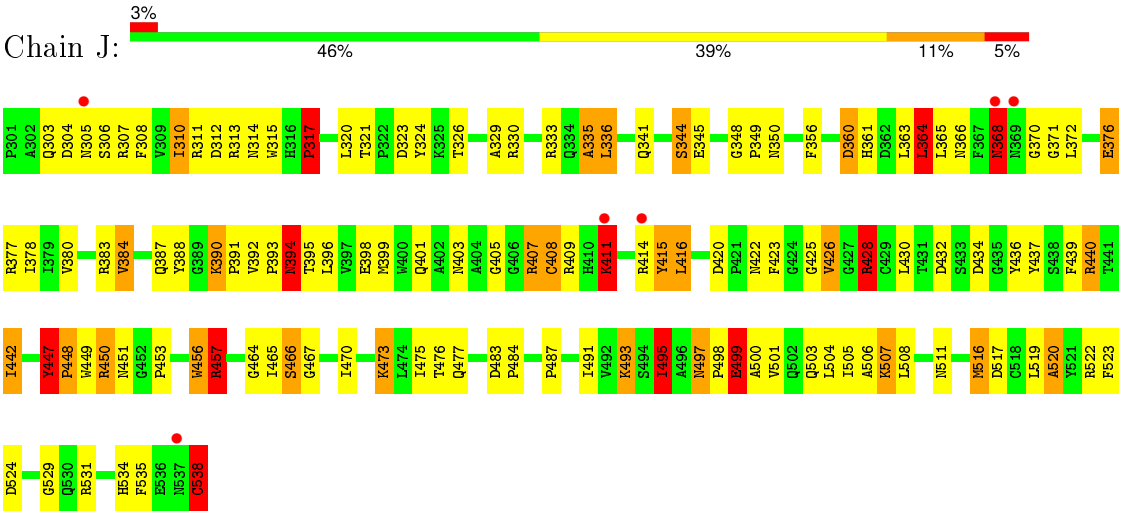
• Molecule 2: Protocatechuate 3,4-dioxygenase beta chain

Chain H:

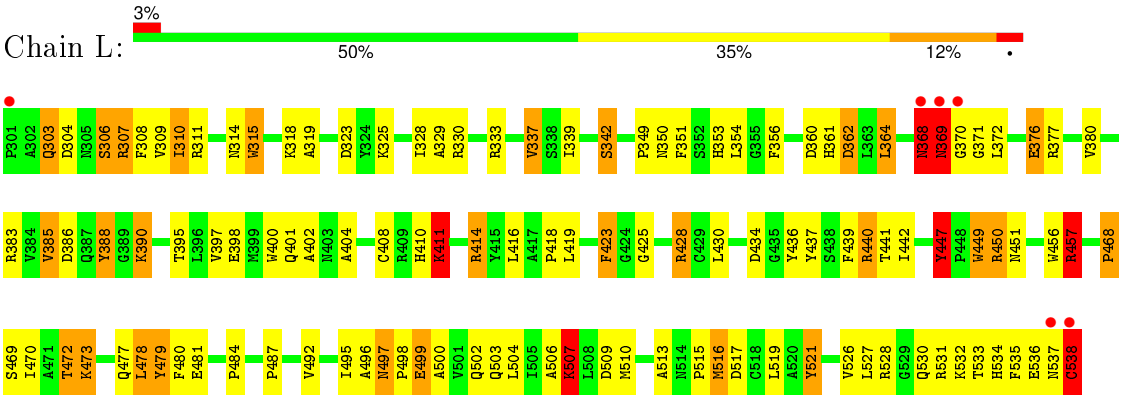




• Molecule 2: Protocatechuate 3,4-dioxygenase beta chain



• Molecule 2: Protocatechuate 3,4-dioxygenase beta chain



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	196.70Å 127.20Å 133.90Å 90.00° 97.60° 90.00°	Depositor
Resolution (Å)	25.64 – 2.25 25.64 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.3 (25.64-2.25) 99.4 (25.64-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.00 (at 1.95Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.158 , 0.199 0.157 , 0.196	Depositor DCC
R_{free} test set	1430 reflections (0.94%)	DCC
Wilson B-factor (Å^2)	32.1	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 38.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.23$	Xtriage
Outliers	1 of 204675 reflections (0.000%)	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	21744	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	2.37	80/1611 (5.0%)	1.77	31/2195 (1.4%)
1	C	2.45	88/1611 (5.5%)	1.88	44/2195 (2.0%)
1	E	2.49	98/1611 (6.1%)	1.85	33/2195 (1.5%)
1	G	2.41	86/1611 (5.3%)	1.86	40/2195 (1.8%)
1	I	2.37	70/1611 (4.3%)	1.81	36/2195 (1.6%)
1	K	2.54	93/1611 (5.8%)	1.82	37/2195 (1.7%)
2	B	2.47	100/1930 (5.2%)	1.89	52/2627 (2.0%)
2	D	2.37	93/1930 (4.8%)	2.03	61/2627 (2.3%)
2	F	2.36	87/1930 (4.5%)	1.92	46/2627 (1.8%)
2	H	2.37	83/1930 (4.3%)	1.92	55/2627 (2.1%)
2	J	2.28	88/1930 (4.6%)	1.88	53/2627 (2.0%)
2	L	2.40	91/1930 (4.7%)	1.86	44/2627 (1.7%)
All	All	2.40	1057/21246 (5.0%)	1.88	532/28932 (1.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	7
1	C	0	10
1	E	0	4
1	G	0	7
1	I	0	7
1	K	0	6
2	B	0	10
2	D	0	15
2	F	0	6
2	H	0	10
2	J	0	16

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	L	0	18
All	All	0	116

All (1057) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	303	GLN	CA-CB	14.72	1.86	1.53
2	D	507	LYS	CE-NZ	14.69	1.85	1.49
2	B	499	GLU	CD-OE1	14.68	1.41	1.25
1	K	168	GLU	CD-OE2	14.48	1.41	1.25
1	C	66	SER	CB-OG	-13.96	1.24	1.42
1	E	47	GLU	CD-OE1	13.79	1.40	1.25
2	B	489	CYS	CB-SG	13.26	2.04	1.82
2	J	447	TYR	CE1-CZ	13.01	1.55	1.38
1	E	192	GLU	CG-CD	12.67	1.71	1.51
1	C	192	GLU	CD-OE2	12.66	1.39	1.25
2	F	499	GLU	CD-OE1	12.60	1.39	1.25
1	I	7	GLU	CD-OE2	12.42	1.39	1.25
2	L	447	TYR	CE1-CZ	12.42	1.54	1.38
2	L	388	TYR	CD2-CE2	12.22	1.57	1.39
1	K	168	GLU	CD-OE1	12.07	1.39	1.25
2	L	538	CYS	CB-SG	-11.94	1.61	1.82
1	A	47	GLU	CD-OE2	11.85	1.38	1.25
2	L	351	PHE	CD2-CE2	11.53	1.62	1.39
1	K	47	GLU	CD-OE2	11.47	1.38	1.25
1	G	16	TYR	CE2-CZ	11.45	1.53	1.38
2	D	426	VAL	CB-CG2	-11.43	1.28	1.52
1	A	157	VAL	CB-CG2	-11.32	1.29	1.52
2	H	436	TYR	CD1-CE1	11.17	1.56	1.39
2	B	507	LYS	CE-NZ	11.15	1.76	1.49
2	L	507	LYS	CE-NZ	11.04	1.76	1.49
2	D	479	TYR	CE2-CZ	-10.97	1.24	1.38
1	E	157	VAL	CB-CG1	10.84	1.75	1.52
1	E	66	SER	CB-OG	-10.77	1.28	1.42
1	C	168	GLU	CD-OE1	10.68	1.37	1.25
2	F	507	LYS	CE-NZ	10.67	1.75	1.49
1	K	78	GLU	CD-OE1	10.63	1.37	1.25
1	K	200	PHE	CE2-CZ	10.57	1.57	1.37
1	C	100	ASP	CB-CG	10.36	1.73	1.51
2	L	337	VAL	CB-CG1	10.36	1.74	1.52
2	L	479	TYR	CD2-CE2	10.31	1.54	1.39
2	B	397	VAL	CB-CG2	-10.30	1.31	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	192	GLU	CG-CD	10.30	1.67	1.51
1	G	176	GLU	CG-CD	10.28	1.67	1.51
2	H	428	ARG	CB-CG	-10.25	1.24	1.52
1	K	86	GLU	CD-OE2	10.23	1.36	1.25
1	A	192	GLU	CG-CD	10.18	1.67	1.51
2	F	437	TYR	CD2-CE2	-10.17	1.24	1.39
1	A	168	GLU	CD-OE1	10.16	1.36	1.25
2	B	479	TYR	CE1-CZ	-10.14	1.25	1.38
2	L	449	TRP	CE3-CZ3	10.14	1.55	1.38
1	I	192	GLU	CD-OE2	10.09	1.36	1.25
1	G	154	LYS	CD-CE	10.07	1.76	1.51
1	A	154	LYS	CE-NZ	10.07	1.74	1.49
1	K	162	GLU	CG-CD	10.05	1.67	1.51
2	F	447	TYR	CE1-CZ	10.03	1.51	1.38
2	L	303	GLN	CA-CB	9.97	1.75	1.53
1	A	192	GLU	CB-CG	9.95	1.71	1.52
2	J	538	CYS	CB-SG	-9.94	1.65	1.82
2	B	398	GLU	CD-OE2	9.92	1.36	1.25
2	B	499	GLU	CD-OE2	9.92	1.36	1.25
2	F	479	TYR	CD2-CE2	9.91	1.54	1.39
1	A	192	GLU	CD-OE2	9.89	1.36	1.25
2	B	502	GLN	CD-OE1	9.88	1.45	1.24
1	I	162	GLU	CD-OE1	9.81	1.36	1.25
1	I	47	GLU	CD-OE2	9.80	1.36	1.25
2	L	531	ARG	CZ-NH1	9.76	1.45	1.33
1	E	16	TYR	CE2-CZ	9.73	1.51	1.38
1	I	7	GLU	CD-OE1	9.71	1.36	1.25
2	J	423	PHE	C-O	9.66	1.41	1.23
1	I	67	PHE	CD1-CE1	9.61	1.58	1.39
1	K	149	ALA	CA-CB	9.54	1.72	1.52
1	K	148	GLU	CD-OE2	9.54	1.36	1.25
1	E	67	PHE	CD1-CE1	9.49	1.58	1.39
1	G	86	GLU	CD-OE1	9.49	1.36	1.25
1	A	154	LYS	CD-CE	9.46	1.74	1.51
1	K	192	GLU	CB-CG	9.46	1.70	1.52
1	G	192	GLU	CB-CG	9.44	1.70	1.52
2	F	436	TYR	CD1-CE1	9.43	1.53	1.39
1	G	71	TRP	CE3-CZ3	9.42	1.54	1.38
2	B	385	VAL	CB-CG1	9.31	1.72	1.52
1	E	176	GLU	CD-OE2	9.31	1.35	1.25
1	I	162	GLU	CD-OE2	9.30	1.35	1.25
1	A	71	TRP	CE3-CZ3	9.27	1.54	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	450	ARG	CZ-NH2	9.27	1.45	1.33
2	J	499	GLU	CG-CD	9.25	1.65	1.51
1	A	47	GLU	CG-CD	9.24	1.65	1.51
1	G	168	GLU	CD-OE2	9.22	1.35	1.25
1	G	188	ARG	CZ-NH1	9.21	1.45	1.33
1	K	78	GLU	CD-OE2	9.20	1.35	1.25
1	A	78	GLU	CD-OE2	9.14	1.35	1.25
2	F	408[A]	CYS	CB-SG	9.14	1.97	1.82
2	F	408[B]	CYS	CB-SG	9.14	1.97	1.82
2	D	521	TYR	CE2-CZ	9.11	1.50	1.38
1	G	69	GLU	CB-CG	-9.10	1.34	1.52
2	H	408[A]	CYS	CB-SG	9.09	1.97	1.82
2	H	408[B]	CYS	CB-SG	9.09	1.97	1.82
1	A	163	GLN	CG-CD	9.05	1.71	1.51
1	C	183	TYR	CD2-CE2	9.05	1.52	1.39
1	I	56	TYR	CD2-CE2	8.99	1.52	1.39
1	A	192	GLU	CD-OE1	8.97	1.35	1.25
2	L	513	ALA	CA-CB	-8.87	1.33	1.52
1	K	83	TYR	CE1-CZ	8.86	1.50	1.38
2	H	499	GLU	CD-OE1	8.83	1.35	1.25
1	K	192	GLU	CG-CD	8.82	1.65	1.51
2	H	479	TYR	CE1-CZ	-8.82	1.27	1.38
1	I	144	TYR	CE2-CZ	8.81	1.50	1.38
1	E	47	GLU	CD-OE2	8.80	1.35	1.25
1	C	3	GLU	CD-OE2	8.79	1.35	1.25
1	G	7	GLU	CB-CG	8.75	1.68	1.52
1	A	3	GLU	CD-OE2	8.74	1.35	1.25
2	F	388	TYR	CD1-CE1	8.74	1.52	1.39
2	H	507	LYS	CD-CE	8.72	1.73	1.51
1	C	154	LYS	CD-CE	8.71	1.73	1.51
1	C	47	GLU	CD-OE2	8.67	1.35	1.25
1	C	120	VAL	CB-CG1	8.63	1.71	1.52
2	F	499	GLU	CG-CD	8.63	1.64	1.51
1	G	47	GLU	CD-OE2	8.63	1.35	1.25
1	C	154	LYS	CE-NZ	8.62	1.70	1.49
1	K	192	GLU	CD-OE2	8.62	1.35	1.25
2	H	538	CYS	CB-SG	-8.61	1.67	1.82
2	J	493	LYS	CE-NZ	8.60	1.70	1.49
1	K	47	GLU	CD-OE1	8.60	1.35	1.25
1	E	197	PHE	CB-CG	-8.59	1.36	1.51
1	K	168	GLU	CG-CD	8.57	1.64	1.51
1	E	3	GLU	CD-OE2	8.56	1.35	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	314	ASN	CB-CG	8.56	1.70	1.51
2	F	450	ARG	CG-CD	8.56	1.73	1.51
1	I	103	GLU	CD-OE1	8.50	1.34	1.25
2	D	367	PHE	CE1-CZ	8.49	1.53	1.37
1	E	16	TYR	CD2-CE2	8.48	1.52	1.39
1	A	3	GLU	CG-CD	8.48	1.64	1.51
1	C	185	PHE	CE2-CZ	-8.47	1.21	1.37
1	E	175	CYS	CB-SG	8.46	1.96	1.82
1	G	3	GLU	CD-OE2	8.42	1.34	1.25
1	G	56	TYR	CD2-CE2	8.42	1.51	1.39
2	D	397	VAL	CB-CG2	-8.41	1.35	1.52
2	H	324	TYR	CE2-CZ	8.40	1.49	1.38
1	G	79	TYR	CG-CD2	8.39	1.50	1.39
1	E	47	GLU	CG-CD	8.38	1.64	1.51
2	H	463	PHE	CD2-CE2	8.37	1.55	1.39
2	J	376	GLU	CD-OE2	8.37	1.34	1.25
1	A	47	GLU	CD-OE1	8.34	1.34	1.25
1	G	79	TYR	CD2-CE2	8.31	1.51	1.39
2	B	330	ARG	CZ-NH2	-8.28	1.22	1.33
1	K	175	CYS	CB-SG	8.28	1.96	1.82
2	F	436	TYR	CG-CD1	8.24	1.49	1.39
2	L	404	ALA	CA-CB	-8.24	1.35	1.52
2	H	388	TYR	CD1-CE1	8.20	1.51	1.39
1	K	3	GLU	CD-OE2	8.20	1.34	1.25
2	D	397	VAL	CB-CG1	-8.18	1.35	1.52
2	F	376	GLU	CD-OE2	8.18	1.34	1.25
2	J	368	ASN	CB-CG	8.14	1.69	1.51
1	G	70	VAL	CB-CG2	-8.13	1.35	1.52
2	H	518	CYS	CB-SG	-8.11	1.68	1.82
2	L	376	GLU	CD-OE1	8.11	1.34	1.25
1	A	99	PHE	CB-CG	8.10	1.65	1.51
1	K	49	ILE	C-O	8.10	1.38	1.23
2	L	308	PHE	CD2-CE2	8.06	1.55	1.39
1	I	144	TYR	CD1-CE1	8.05	1.51	1.39
2	D	499	GLU	CD-OE1	8.04	1.34	1.25
2	H	475	ILE	CG1-CD1	-8.03	0.95	1.50
1	I	176	GLU	CG-CD	8.03	1.64	1.51
2	H	436	TYR	CD2-CE2	8.02	1.51	1.39
1	G	176	GLU	CD-OE2	8.01	1.34	1.25
2	F	303	GLN	CA-CB	8.01	1.71	1.53
2	H	303	GLN	CA-CB	8.00	1.71	1.53
1	C	136	ASN	C-O	8.00	1.38	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	183	TYR	CE1-CZ	8.00	1.49	1.38
1	I	47	GLU	CD-OE1	7.99	1.34	1.25
2	D	408[A]	CYS	CB-SG	7.98	1.95	1.82
2	D	408[B]	CYS	CB-SG	7.98	1.95	1.82
1	I	168	GLU	CD-OE1	7.98	1.34	1.25
1	E	103	GLU	CD-OE1	7.97	1.34	1.25
2	F	535	PHE	CG-CD2	7.97	1.50	1.38
1	G	192	GLU	CD-OE2	7.96	1.34	1.25
1	I	154	LYS	CE-NZ	7.94	1.68	1.49
2	H	309	VAL	CB-CG1	7.92	1.69	1.52
1	E	73	ALA	CA-CB	-7.90	1.35	1.52
2	B	408[A]	CYS	CB-SG	7.87	1.95	1.82
2	B	408[B]	CYS	CB-SG	7.87	1.95	1.82
2	L	383	ARG	CZ-NH1	7.87	1.43	1.33
1	E	200	PHE	CG-CD1	7.87	1.50	1.38
1	E	92	PHE	CE1-CZ	7.85	1.52	1.37
2	H	358	ALA	CA-CB	7.85	1.69	1.52
1	K	162	GLU	CD-OE2	7.83	1.34	1.25
1	E	162	GLU	CG-CD	7.83	1.63	1.51
1	K	192	GLU	CD-OE1	7.83	1.34	1.25
2	B	447	TYR	CE1-CZ	7.83	1.48	1.38
2	H	436	TYR	CE2-CZ	7.82	1.48	1.38
1	G	7	GLU	CD-OE2	7.81	1.34	1.25
1	G	165	GLN	CG-CD	7.80	1.69	1.51
1	G	168	GLU	CD-OE1	7.79	1.34	1.25
1	C	64	ARG	CZ-NH1	7.79	1.43	1.33
2	F	333	ARG	CZ-NH2	7.77	1.43	1.33
2	J	380	VAL	CB-CG2	7.77	1.69	1.52
1	C	16	TYR	CE2-CZ	7.77	1.48	1.38
2	D	493	LYS	CE-NZ	7.76	1.68	1.49
1	K	103	GLU	CD-OE1	7.73	1.34	1.25
2	L	402	ALA	CA-CB	7.73	1.68	1.52
2	L	499	GLU	CD-OE1	7.72	1.34	1.25
1	K	13	ALA	C-O	7.72	1.38	1.23
2	L	507	LYS	CD-CE	7.71	1.70	1.51
1	E	99	PHE	CD1-CE1	7.70	1.54	1.39
2	J	499	GLU	CD-OE1	7.70	1.34	1.25
2	H	354	LEU	C-O	7.70	1.38	1.23
1	G	192	GLU	CG-CD	7.69	1.63	1.51
1	G	3	GLU	CD-OE1	7.69	1.34	1.25
2	B	480	PHE	CE2-CZ	7.68	1.51	1.37
2	J	324	TYR	CE2-CZ	7.67	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	86	GLU	CG-CD	7.62	1.63	1.51
2	D	342	SER	CB-OG	7.62	1.52	1.42
1	C	71	TRP	C-O	7.62	1.37	1.23
2	F	535	PHE	CE2-CZ	7.62	1.51	1.37
1	K	66	SER	CB-OG	-7.62	1.32	1.42
2	F	390	LYS	CG-CD	7.61	1.78	1.52
1	A	162	GLU	CG-CD	7.61	1.63	1.51
2	H	329	ALA	CA-CB	-7.58	1.36	1.52
1	G	9	PRO	CG-CD	7.56	1.75	1.50
1	C	99	PHE	CD1-CE1	7.55	1.54	1.39
2	F	385	VAL	CB-CG1	-7.54	1.37	1.52
2	D	449	TRP	CE3-CZ3	7.54	1.51	1.38
2	J	388	TYR	CD1-CE1	7.54	1.50	1.39
1	K	99	PHE	CE2-CZ	7.54	1.51	1.37
1	E	192	GLU	CB-CG	7.53	1.66	1.52
1	C	133	ARG	CB-CG	-7.52	1.32	1.52
1	K	64	ARG	CZ-NH1	7.49	1.42	1.33
2	D	481	GLU	CD-OE1	-7.48	1.17	1.25
2	B	388	TYR	CD1-CE1	7.47	1.50	1.39
1	K	103	GLU	CG-CD	7.46	1.63	1.51
1	A	120	VAL	CB-CG1	7.46	1.68	1.52
1	C	16	TYR	CZ-OH	7.46	1.50	1.37
1	G	3	GLU	CG-CD	7.45	1.63	1.51
1	E	78	GLU	CD-OE2	7.44	1.33	1.25
2	L	481	GLU	CD-OE1	-7.44	1.17	1.25
1	C	157	VAL	CB-CG2	-7.42	1.37	1.52
1	E	198	PHE	CD1-CE1	7.42	1.54	1.39
1	E	192	GLU	CD-OE1	7.42	1.33	1.25
1	E	16	TYR	CE1-CZ	7.42	1.48	1.38
1	C	83	TYR	CZ-OH	-7.40	1.25	1.37
1	I	155	CYS	CB-SG	7.39	1.94	1.82
1	I	7	GLU	CB-CG	7.39	1.66	1.52
1	G	56	TYR	CE1-CZ	7.39	1.48	1.38
1	I	47	GLU	CG-CD	7.38	1.63	1.51
2	L	447	TYR	CB-CG	-7.37	1.40	1.51
2	L	499	GLU	CD-OE2	7.37	1.33	1.25
2	J	456	TRP	CG-CD1	7.36	1.47	1.36
1	A	67	PHE	CE1-CZ	7.36	1.51	1.37
2	D	376	GLU	CD-OE1	7.36	1.33	1.25
2	H	396	LEU	CG-CD1	7.35	1.79	1.51
2	D	325	LYS	CE-NZ	-7.34	1.30	1.49
2	B	368	ASN	CB-CG	7.33	1.68	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	144	TYR	CB-CG	-7.32	1.40	1.51
1	C	180	LYS	CE-NZ	7.32	1.67	1.49
1	C	67	PHE	CB-CG	-7.31	1.39	1.51
2	J	333	ARG	CG-CD	7.28	1.70	1.51
1	E	182	ALA	CA-CB	-7.27	1.37	1.52
2	B	536	GLU	CG-CD	-7.27	1.41	1.51
1	E	71	TRP	CB-CG	-7.27	1.37	1.50
1	C	69	GLU	CB-CG	-7.26	1.38	1.52
1	C	168	GLU	CG-CD	7.26	1.62	1.51
1	I	198	PHE	CE2-CZ	7.24	1.51	1.37
2	L	380	VAL	CA-CB	7.24	1.70	1.54
2	D	366	ASN	C-O	-7.24	1.09	1.23
2	J	457	ARG	CZ-NH2	7.23	1.42	1.33
2	F	522	ARG	CG-CD	-7.21	1.33	1.51
2	B	392	VAL	CB-CG2	7.21	1.68	1.52
2	H	321	THR	C-O	7.21	1.37	1.23
2	F	520	ALA	CA-CB	-7.21	1.37	1.52
1	I	154	LYS	CD-CE	7.20	1.69	1.51
1	G	80	GLN	CG-CD	7.19	1.67	1.51
2	L	516	MET	CG-SD	7.19	1.99	1.81
2	L	383	ARG	CZ-NH2	7.18	1.42	1.33
2	J	415	TYR	CG-CD2	7.18	1.48	1.39
1	E	78	GLU	CD-OE1	7.17	1.33	1.25
1	E	177	VAL	CB-CG1	7.17	1.67	1.52
2	H	400	TRP	CB-CG	-7.15	1.37	1.50
1	I	105	THR	CA-CB	7.15	1.72	1.53
1	C	192	GLU	CG-CD	7.14	1.62	1.51
1	I	3	GLU	CD-OE2	7.14	1.33	1.25
2	H	330	ARG	CZ-NH2	7.13	1.42	1.33
1	I	92	PHE	CG-CD2	7.12	1.49	1.38
1	E	11	GLN	N-CA	7.11	1.60	1.46
2	D	450	ARG	CZ-NH1	7.09	1.42	1.33
1	K	174	ARG	CZ-NH1	7.08	1.42	1.33
1	C	99	PHE	CD2-CE2	7.08	1.53	1.39
2	D	453	PRO	CA-CB	-7.07	1.39	1.53
2	B	499	GLU	CG-CD	7.06	1.62	1.51
1	A	99	PHE	CE1-CZ	7.05	1.50	1.37
1	G	47	GLU	CD-OE1	7.04	1.33	1.25
2	B	506	ALA	CA-CB	-7.04	1.37	1.52
2	L	369	ASN	C-O	7.04	1.36	1.23
2	F	480	PHE	CD1-CE1	7.04	1.53	1.39
2	D	383	ARG	CB-CG	-7.04	1.33	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	56	TYR	CE1-CZ	7.03	1.47	1.38
1	I	99	PHE	CE2-CZ	7.02	1.50	1.37
1	I	99	PHE	CD2-CE2	7.00	1.53	1.39
2	L	333	ARG	CG-CD	7.00	1.69	1.51
1	I	150	GLN	CG-CD	7.00	1.67	1.51
1	C	114	VAL	CB-CG2	-6.99	1.38	1.52
2	D	510	MET	SD-CE	6.99	2.17	1.77
1	I	197	PHE	CE1-CZ	6.99	1.50	1.37
2	L	351	PHE	CE2-CZ	-6.98	1.24	1.37
1	E	192	GLU	CD-OE2	6.97	1.33	1.25
2	L	436	TYR	CD1-CE1	6.97	1.49	1.39
2	D	376	GLU	CD-OE2	6.96	1.33	1.25
1	G	16	TYR	CB-CG	6.96	1.62	1.51
1	K	133	ARG	CZ-NH2	6.96	1.42	1.33
2	L	502	GLN	CD-OE1	6.96	1.39	1.24
1	I	89	PHE	CE1-CZ	-6.95	1.24	1.37
2	F	500	ALA	CA-CB	-6.94	1.37	1.52
1	I	16	TYR	CE2-CZ	6.94	1.47	1.38
2	L	436	TYR	CD2-CE2	6.94	1.49	1.39
2	D	303	GLN	CA-CB	6.94	1.69	1.53
2	J	450	ARG	CZ-NH1	6.93	1.42	1.33
1	K	183	TYR	CG-CD2	6.93	1.48	1.39
2	B	383	ARG	CZ-NH2	6.93	1.42	1.33
2	L	457	ARG	CZ-NH1	6.92	1.42	1.33
2	J	414	ARG	CG-CD	6.91	1.69	1.51
2	F	411	LYS	CE-NZ	6.91	1.66	1.49
2	J	311	ARG	CZ-NH1	-6.91	1.24	1.33
1	A	178	ASP	CB-CG	6.89	1.66	1.51
2	L	385	VAL	C-O	6.89	1.36	1.23
2	L	351	PHE	CE1-CZ	6.89	1.50	1.37
2	L	439	PHE	CE1-CZ	6.88	1.50	1.37
1	E	70	VAL	CB-CG1	-6.88	1.38	1.52
1	K	67	PHE	CE2-CZ	6.88	1.50	1.37
1	I	192	GLU	CD-OE1	6.88	1.33	1.25
1	C	177	VAL	CB-CG2	-6.87	1.38	1.52
2	J	531	ARG	CZ-NH1	6.87	1.42	1.33
2	D	520	ALA	CA-CB	-6.87	1.38	1.52
2	D	414	ARG	CZ-NH1	6.87	1.42	1.33
2	B	449	TRP	CG-CD1	6.86	1.46	1.36
2	F	383	ARG	CB-CG	-6.86	1.34	1.52
1	A	91	SER	CA-CB	-6.86	1.42	1.52
2	B	453	PRO	CG-CD	6.86	1.73	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	503	GLN	CD-OE1	6.85	1.39	1.24
2	J	507	LYS	CE-NZ	6.85	1.66	1.49
2	H	437	TYR	CG-CD1	6.85	1.48	1.39
2	H	377	ARG	CB-CG	6.85	1.71	1.52
2	L	480	PHE	CE1-CZ	6.85	1.50	1.37
2	L	354	LEU	C-O	6.84	1.36	1.23
1	K	86	GLU	CD-OE1	6.84	1.33	1.25
2	H	447	TYR	CD2-CE2	6.83	1.49	1.39
2	L	521	TYR	CE2-CZ	6.83	1.47	1.38
1	E	83	TYR	CG-CD1	6.83	1.48	1.39
2	H	507	LYS	CE-NZ	6.83	1.66	1.49
2	J	303	GLN	CA-CB	6.83	1.69	1.53
1	K	166	ARG	CG-CD	6.83	1.69	1.51
2	B	390	LYS	CD-CE	6.83	1.68	1.51
2	L	531	ARG	CZ-NH2	6.82	1.42	1.33
1	A	131	PHE	CE2-CZ	6.82	1.50	1.37
2	J	333	ARG	CZ-NH1	6.81	1.42	1.33
2	D	502	GLN	CG-CD	6.81	1.66	1.51
2	F	457	ARG	CZ-NH1	6.81	1.41	1.33
1	C	3	GLU	CD-OE1	6.80	1.33	1.25
2	D	436	TYR	CE2-CZ	6.80	1.47	1.38
1	G	176	GLU	CD-OE1	6.80	1.33	1.25
2	B	457	ARG	CD-NE	6.79	1.57	1.46
1	E	90	ASN	C-O	6.79	1.36	1.23
2	B	507	LYS	CD-CE	6.79	1.68	1.51
2	D	505	ILE	CA-CB	-6.79	1.39	1.54
1	E	103	GLU	CG-CD	6.79	1.62	1.51
1	C	99	PHE	CE1-CZ	6.78	1.50	1.37
1	K	188	ARG	CG-CD	6.78	1.69	1.51
1	G	130	LEU	C-O	6.78	1.36	1.23
1	I	69	GLU	CD-OE2	6.78	1.33	1.25
2	B	388	TYR	CD2-CE2	6.78	1.49	1.39
1	I	86	GLU	CD-OE1	6.78	1.33	1.25
2	L	469	SER	CA-CB	6.77	1.63	1.52
1	A	63	VAL	CA-CB	-6.76	1.40	1.54
2	F	423	PHE	CD1-CE1	-6.76	1.25	1.39
2	D	423	PHE	CE1-CZ	6.75	1.50	1.37
1	A	120	VAL	CB-CG2	-6.75	1.38	1.52
1	E	99	PHE	CB-CG	6.73	1.62	1.51
2	D	480	PHE	CB-CG	-6.73	1.40	1.51
1	K	144	TYR	CE2-CZ	6.72	1.47	1.38
2	L	472	THR	CB-CG2	-6.72	1.30	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	324	TYR	CG-CD1	6.72	1.47	1.39
2	H	436	TYR	CB-CG	-6.71	1.41	1.51
2	B	377	ARG	CZ-NH1	6.71	1.41	1.33
1	G	104	TRP	CZ3-CH2	6.71	1.50	1.40
2	J	409	ARG	CA-C	6.70	1.70	1.52
2	D	411	LYS	CD-CE	6.70	1.68	1.51
2	F	450	ARG	CZ-NH2	6.70	1.41	1.33
1	C	200	PHE	CD1-CE1	6.70	1.52	1.39
2	D	330	ARG	CZ-NH2	6.69	1.41	1.33
2	H	480	PHE	CG-CD2	6.69	1.48	1.38
2	J	523	PHE	CE1-CZ	6.69	1.50	1.37
1	K	145	PHE	CD1-CE1	6.69	1.52	1.39
2	D	411	LYS	CE-NZ	6.69	1.65	1.49
2	F	375	GLY	C-O	-6.68	1.12	1.23
1	I	93	GLY	C-O	6.68	1.34	1.23
2	B	493	LYS	CD-CE	6.68	1.68	1.51
2	B	390	LYS	CE-NZ	6.67	1.65	1.49
2	J	329	ALA	CA-CB	-6.67	1.38	1.52
2	J	390	LYS	CE-NZ	6.67	1.65	1.49
1	A	66	SER	CB-OG	-6.66	1.33	1.42
1	I	103	GLU	CG-CD	6.66	1.61	1.51
1	C	188	ARG	CZ-NH1	6.65	1.41	1.33
2	H	377	ARG	C-O	6.65	1.35	1.23
2	L	436	TYR	CE2-CZ	6.64	1.47	1.38
1	I	194	GLU	CB-CG	-6.63	1.39	1.52
1	K	168	GLU	CB-CG	6.63	1.64	1.52
1	E	69	GLU	CD-OE2	6.63	1.32	1.25
1	G	67	PHE	CG-CD2	-6.63	1.28	1.38
1	G	103	GLU	CD-OE1	6.62	1.32	1.25
1	C	98	THR	N-CA	6.62	1.59	1.46
2	D	368	ASN	CB-CG	6.62	1.66	1.51
2	B	440	ARG	CZ-NH1	6.61	1.41	1.33
2	B	521	TYR	CD2-CE2	6.61	1.49	1.39
1	K	52	LEU	C-O	6.59	1.35	1.23
2	H	526	VAL	CB-CG2	6.59	1.66	1.52
1	E	99	PHE	CD2-CE2	6.58	1.52	1.39
2	L	499	GLU	CG-CD	6.58	1.61	1.51
2	L	450	ARG	CZ-NH2	6.58	1.41	1.33
1	C	24	GLU	CG-CD	6.57	1.61	1.51
2	D	333	ARG	CZ-NH2	6.57	1.41	1.33
2	J	377	ARG	CZ-NH2	6.57	1.41	1.33
1	E	9	PRO	CG-CD	6.56	1.72	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	118	ALA	CA-CB	6.56	1.66	1.52
2	D	481	GLU	CB-CG	-6.55	1.39	1.52
2	J	535	PHE	CE2-CZ	6.55	1.49	1.37
2	B	366	ASN	CB-CG	6.54	1.66	1.51
1	I	67	PHE	CE2-CZ	6.54	1.49	1.37
1	G	99	PHE	CD1-CE1	6.54	1.52	1.39
1	E	188	ARG	NE-CZ	6.53	1.41	1.33
1	E	185	PHE	CD1-CE1	6.52	1.52	1.39
2	H	502	GLN	CD-OE1	6.52	1.38	1.24
1	A	89	PHE	CE1-CZ	6.52	1.49	1.37
2	L	339	ILE	C-O	6.51	1.35	1.23
2	B	434	ASP	N-CA	-6.51	1.33	1.46
2	F	368	ASN	CB-CG	6.51	1.66	1.51
1	I	38	ARG	CZ-NH1	6.51	1.41	1.33
2	H	351	PHE	CE1-CZ	-6.50	1.25	1.37
1	A	56	TYR	CD2-CE2	6.50	1.49	1.39
1	I	99	PHE	CE1-CZ	6.50	1.49	1.37
2	H	521	TYR	CE1-CZ	6.50	1.47	1.38
2	F	450	ARG	CZ-NH1	6.49	1.41	1.33
1	E	163	GLN	CD-OE1	6.49	1.38	1.24
2	F	436	TYR	CD2-CE2	6.49	1.49	1.39
1	C	86	GLU	CD-OE2	6.49	1.32	1.25
2	F	481	GLU	CD-OE1	-6.49	1.18	1.25
2	H	368	ASN	CB-CG	6.47	1.66	1.51
1	K	3	GLU	CG-CD	6.47	1.61	1.51
1	E	11	GLN	CD-NE2	-6.47	1.16	1.32
1	G	176	GLU	CB-CG	6.47	1.64	1.52
1	G	185	PHE	CE1-CZ	6.47	1.49	1.37
2	D	499	GLU	CG-CD	6.47	1.61	1.51
2	F	426	VAL	C-O	6.46	1.35	1.23
1	C	168	GLU	CD-OE2	6.46	1.32	1.25
1	I	16	TYR	CZ-OH	6.46	1.48	1.37
2	J	345	GLU	CB-CG	-6.46	1.39	1.52
1	K	196	VAL	C-O	6.46	1.35	1.23
1	A	34	GLU	CD-OE2	-6.45	1.18	1.25
1	G	183	TYR	CD2-CE2	6.45	1.49	1.39
1	A	44	ALA	CA-CB	6.44	1.66	1.52
2	B	394	ASN	C-O	-6.44	1.11	1.23
2	L	318	LYS	CD-CE	6.44	1.67	1.51
2	H	461	ILE	C-O	6.44	1.35	1.23
2	F	349	PRO	CA-C	-6.43	1.40	1.52
1	E	150	GLN	CG-CD	6.43	1.65	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	97	THR	C-O	6.42	1.35	1.23
1	C	184	ARG	N-CA	-6.42	1.33	1.46
2	L	356	PHE	CE2-CZ	6.42	1.49	1.37
1	G	64	ARG	CZ-NH1	6.42	1.41	1.33
1	E	188	ARG	CG-CD	6.41	1.68	1.51
2	J	390	LYS	CG-CD	6.41	1.74	1.52
2	B	301	PRO	C-O	6.41	1.36	1.23
2	D	351	PHE	CE2-CZ	6.41	1.49	1.37
1	A	99	PHE	CG-CD1	6.40	1.48	1.38
2	J	390	LYS	CD-CE	6.39	1.67	1.51
1	C	10	SER	CB-OG	-6.39	1.33	1.42
1	K	41	LYS	CD-CE	6.39	1.67	1.51
2	D	390	LYS	CD-CE	6.38	1.67	1.51
2	J	439	PHE	CE2-CZ	6.38	1.49	1.37
1	G	76	ASN	CG-OD1	6.38	1.38	1.24
2	J	414	ARG	CZ-NH1	6.37	1.41	1.33
1	E	144	TYR	CZ-OH	6.37	1.48	1.37
1	C	47	GLU	CD-OE1	6.37	1.32	1.25
1	A	13	ALA	CA-CB	-6.36	1.39	1.52
2	F	437	TYR	CE2-CZ	6.35	1.46	1.38
1	K	188	ARG	CZ-NH1	6.35	1.41	1.33
1	A	144	TYR	CZ-OH	6.33	1.48	1.37
2	B	438	SER	CB-OG	-6.33	1.34	1.42
1	G	25	ALA	CA-CB	6.32	1.65	1.52
2	H	493	LYS	CE-NZ	6.32	1.64	1.49
2	D	493	LYS	CD-CE	6.31	1.67	1.51
2	J	411	LYS	CD-CE	6.31	1.67	1.51
2	L	479	TYR	C-O	6.30	1.35	1.23
2	D	436	TYR	CD2-CE2	6.29	1.48	1.39
1	K	99	PHE	CG-CD2	6.29	1.48	1.38
2	D	454	ASN	C-O	-6.28	1.11	1.23
1	I	142	ARG	CZ-NH1	6.27	1.41	1.33
1	C	70	VAL	CB-CG1	6.27	1.66	1.52
1	G	122	MET	SD-CE	-6.25	1.42	1.77
1	A	103	GLU	CG-CD	6.25	1.61	1.51
1	C	171	ILE	CB-CG2	-6.24	1.33	1.52
2	D	368	ASN	CA-CB	6.23	1.69	1.53
2	B	450	ARG	CZ-NH2	6.23	1.41	1.33
2	B	436	TYR	CD1-CE1	6.23	1.48	1.39
1	E	174	ARG	CZ-NH1	6.23	1.41	1.33
2	H	428	ARG	CZ-NH2	6.23	1.41	1.33
2	B	329	ALA	CA-CB	-6.22	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	499	GLU	CD-OE2	6.22	1.32	1.25
1	E	70	VAL	CB-CG2	-6.22	1.39	1.52
2	B	333	ARG	CZ-NH1	6.22	1.41	1.33
2	L	536	GLU	CD-OE1	6.22	1.32	1.25
2	L	532	LYS	CA-CB	6.21	1.67	1.53
2	H	385	VAL	CB-CG1	6.21	1.65	1.52
2	F	524	ASP	C-O	-6.21	1.11	1.23
1	A	129	SER	N-CA	-6.21	1.33	1.46
1	A	194	GLU	CG-CD	6.20	1.61	1.51
2	D	447	TYR	CE1-CZ	6.20	1.46	1.38
2	H	501	VAL	CB-CG2	6.20	1.65	1.52
2	B	495	ILE	CG1-CD1	-6.19	1.07	1.50
2	F	430	LEU	C-O	-6.19	1.11	1.23
2	D	437	TYR	CG-CD2	-6.18	1.31	1.39
1	E	26	ALA	CA-CB	6.17	1.65	1.52
1	A	101	ALA	C-N	6.17	1.44	1.33
2	L	318	LYS	CE-NZ	6.17	1.64	1.49
1	K	69	GLU	CD-OE2	6.17	1.32	1.25
2	B	315	TRP	CZ2-CH2	6.16	1.49	1.37
2	H	447	TYR	CE1-CZ	6.15	1.46	1.38
1	I	192	GLU	CB-CG	6.15	1.63	1.52
2	L	439	PHE	CG-CD1	6.15	1.48	1.38
1	C	84	ASN	CB-CG	6.15	1.65	1.51
2	F	443	LYS	CE-NZ	6.14	1.64	1.49
2	B	327	SER	N-CA	-6.14	1.34	1.46
1	G	183	TYR	CB-CG	-6.14	1.42	1.51
1	G	99	PHE	CE1-CZ	6.13	1.49	1.37
1	G	132	ALA	CA-CB	-6.13	1.39	1.52
1	C	162	GLU	CD-OE1	6.13	1.32	1.25
1	E	198	PHE	CD2-CE2	6.12	1.51	1.39
2	J	448	PRO	CB-CG	6.12	1.80	1.50
2	J	456	TRP	CZ3-CH2	6.12	1.49	1.40
1	K	92	PHE	CE1-CZ	6.12	1.49	1.37
1	G	99	PHE	CD2-CE2	6.12	1.51	1.39
2	B	365	LEU	C-O	-6.10	1.11	1.23
2	F	426	VAL	CB-CG2	-6.10	1.40	1.52
1	E	176	GLU	CG-CD	6.10	1.61	1.51
2	F	480	PHE	CE1-CZ	-6.10	1.25	1.37
1	C	16	TYR	CE1-CZ	6.09	1.46	1.38
1	A	200	PHE	CD2-CE2	6.09	1.51	1.39
2	D	407	ARG	N-CA	6.09	1.58	1.46
1	A	36	TRP	CB-CG	6.09	1.61	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	522	ARG	CZ-NH2	6.08	1.41	1.33
1	C	73	ALA	CA-CB	-6.08	1.39	1.52
2	L	414	ARG	NE-CZ	6.07	1.41	1.33
2	J	436	TYR	CD2-CE2	6.07	1.48	1.39
2	L	370	GLY	C-O	6.06	1.33	1.23
2	B	493	LYS	CE-NZ	6.06	1.64	1.49
2	D	440	ARG	CG-CD	-6.06	1.36	1.51
1	C	103	GLU	CD-OE2	6.06	1.32	1.25
1	K	17	VAL	C-O	6.05	1.34	1.23
1	A	83	TYR	CD1-CE1	-6.05	1.30	1.39
2	H	414	ARG	CB-CG	6.05	1.68	1.52
1	C	71	TRP	CZ3-CH2	-6.04	1.30	1.40
1	A	103	GLU	CD-OE1	6.04	1.32	1.25
2	D	414	ARG	CB-CG	6.04	1.68	1.52
2	J	466	SER	CB-OG	6.03	1.50	1.42
2	L	535	PHE	CE2-CZ	6.03	1.48	1.37
1	C	56	TYR	CZ-OH	6.03	1.48	1.37
1	C	14	GLY	CA-C	6.02	1.61	1.51
2	F	411	LYS	CD-CE	6.02	1.66	1.51
2	H	499	GLU	CD-OE2	6.02	1.32	1.25
2	J	436	TYR	CE2-CZ	6.01	1.46	1.38
1	E	176	GLU	CB-CG	6.01	1.63	1.52
2	F	331	SER	C-O	-6.01	1.11	1.23
1	A	198	PHE	CD1-CE1	6.00	1.51	1.39
1	K	198	PHE	CG-CD1	6.00	1.47	1.38
2	L	473	LYS	CE-NZ	6.00	1.64	1.49
2	D	535	PHE	CD1-CE1	6.00	1.51	1.39
1	A	113	VAL	CB-CG1	5.99	1.65	1.52
2	L	447	TYR	CD1-CE1	5.99	1.48	1.39
2	L	528	ARG	CG-CD	5.99	1.67	1.51
1	A	196	VAL	CB-CG2	-5.98	1.40	1.52
1	C	144	TYR	CD2-CE2	-5.97	1.30	1.39
1	E	183	TYR	C-O	-5.97	1.12	1.23
1	E	150	GLN	CD-OE1	5.97	1.37	1.24
1	E	168	GLU	CD-OE1	5.97	1.32	1.25
1	E	176	GLU	CD-OE1	5.97	1.32	1.25
1	G	54	GLN	CD-OE1	5.96	1.37	1.24
2	L	397	VAL	CB-CG2	5.96	1.65	1.52
2	H	436	TYR	CG-CD1	5.95	1.46	1.39
1	I	53	GLY	C-O	5.95	1.33	1.23
2	B	351	PHE	CE2-CZ	5.95	1.48	1.37
2	L	418	PRO	CA-C	-5.94	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	380	VAL	CB-CG2	-5.94	1.40	1.52
1	K	38	ARG	CB-CG	5.93	1.68	1.52
2	F	449	TRP	CZ3-CH2	5.93	1.49	1.40
1	K	155	CYS	CB-SG	5.93	1.92	1.82
2	L	437	TYR	CB-CG	-5.93	1.42	1.51
2	F	437	TYR	CD1-CE1	5.93	1.48	1.39
2	H	498	PRO	CB-CG	5.93	1.79	1.50
2	L	496	ALA	CA-CB	5.92	1.64	1.52
2	H	383	ARG	CB-CG	-5.92	1.36	1.52
1	G	131	PHE	CE2-CZ	5.92	1.48	1.37
1	A	197	PHE	CE2-CZ	5.92	1.48	1.37
1	G	185	PHE	CG-CD2	5.92	1.47	1.38
1	E	162	GLU	CD-OE1	5.92	1.32	1.25
1	E	38	ARG	NE-CZ	5.91	1.40	1.33
1	E	158	LEU	C-O	-5.91	1.12	1.23
2	H	311	ARG	CA-CB	-5.91	1.41	1.53
2	F	493	LYS	CG-CD	5.91	1.72	1.52
1	I	165	GLN	CG-CD	5.91	1.64	1.51
2	J	439	PHE	CG-CD1	5.91	1.47	1.38
2	J	477	GLN	CD-OE1	5.90	1.36	1.24
1	C	71	TRP	CE3-CZ3	5.90	1.48	1.38
1	E	89	PHE	CE2-CZ	5.90	1.48	1.37
1	A	99	PHE	CG-CD2	5.90	1.47	1.38
1	A	145	PHE	CD2-CE2	5.89	1.51	1.39
1	C	131	PHE	CE1-CZ	-5.89	1.26	1.37
1	E	89	PHE	CB-CG	-5.89	1.41	1.51
1	G	2	ILE	CG1-CD1	-5.88	1.09	1.50
2	J	376	GLU	CD-OE1	5.88	1.32	1.25
1	K	83	TYR	CE2-CZ	5.88	1.46	1.38
1	G	133	ARG	NE-CZ	5.88	1.40	1.33
2	H	463	PHE	CD1-CE1	5.88	1.50	1.39
2	L	342	SER	CB-OG	5.88	1.49	1.42
1	A	114	VAL	C-O	5.87	1.34	1.23
2	B	400	TRP	CZ3-CH2	5.87	1.49	1.40
1	A	200	PHE	CD1-CE1	5.86	1.50	1.39
2	B	363	LEU	C-O	-5.86	1.12	1.23
2	J	326	THR	C-O	-5.86	1.12	1.23
2	B	306	SER	CB-OG	-5.86	1.34	1.42
2	L	423	PHE	CD1-CE1	5.85	1.50	1.39
1	G	161	ILE	C-O	-5.85	1.12	1.23
1	E	80	GLN	CD-OE1	5.85	1.36	1.24
1	E	109	VAL	CB-CG2	-5.85	1.40	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	423	PHE	CE1-CZ	5.84	1.48	1.37
2	H	337	VAL	CB-CG1	5.82	1.65	1.52
1	I	174	ARG	CZ-NH2	5.82	1.40	1.33
1	G	197	PHE	CE1-CZ	-5.82	1.26	1.37
1	G	198	PHE	CD1-CE1	5.82	1.50	1.39
1	I	82	ALA	CA-CB	5.82	1.64	1.52
1	E	79	TYR	CE1-CZ	5.82	1.46	1.38
2	F	388	TYR	CD2-CE2	5.82	1.48	1.39
2	J	503	GLN	CG-CD	5.81	1.64	1.51
1	C	63	VAL	CB-CG2	-5.81	1.40	1.52
2	H	514	ASN	C-O	-5.81	1.12	1.23
1	I	198	PHE	CD2-CE2	5.81	1.50	1.39
1	K	115	ASN	CB-CG	5.81	1.64	1.51
1	E	166	ARG	CZ-NH2	5.80	1.40	1.33
2	F	342	SER	CB-OG	5.80	1.49	1.42
2	B	320	LEU	N-CA	5.80	1.57	1.46
2	B	411	LYS	CD-CE	5.80	1.65	1.51
1	G	132	ALA	C-O	5.80	1.34	1.23
2	D	522	ARG	CB-CG	-5.80	1.36	1.52
1	E	7	GLU	CD-OE2	5.80	1.32	1.25
2	D	430	LEU	C-O	-5.79	1.12	1.23
1	I	168	GLU	CD-OE2	5.79	1.32	1.25
2	B	530	GLN	C-O	-5.79	1.12	1.23
2	H	471	ALA	N-CA	5.79	1.57	1.46
2	L	368	ASN	CB-CG	5.79	1.64	1.51
2	J	411	LYS	CB-CG	5.78	1.68	1.52
2	B	398	GLU	C-O	5.77	1.34	1.23
1	E	64	ARG	CZ-NH1	5.77	1.40	1.33
2	J	426	VAL	CB-CG1	5.77	1.65	1.52
2	H	367	PHE	CE2-CZ	5.77	1.48	1.37
2	D	409	ARG	CB-CG	-5.77	1.36	1.52
1	A	198	PHE	CE2-CZ	5.76	1.48	1.37
1	E	56	TYR	CB-CG	-5.76	1.43	1.51
1	G	137	ILE	N-CA	-5.76	1.34	1.46
2	J	470	ILE	CB-CG2	5.76	1.70	1.52
2	H	449	TRP	CE3-CZ3	5.75	1.48	1.38
1	I	146	ASP	CG-OD2	5.75	1.38	1.25
1	K	99	PHE	CG-CD1	5.75	1.47	1.38
2	F	311	ARG	CA-CB	-5.75	1.41	1.53
2	J	522	ARG	CB-CG	-5.75	1.37	1.52
2	J	384	VAL	CB-CG1	-5.74	1.40	1.52
1	C	109	VAL	CB-CG2	-5.74	1.40	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	521	TYR	CD1-CE1	5.74	1.48	1.39
2	F	454	ASN	C-O	-5.74	1.12	1.23
1	K	114	VAL	CA-CB	5.74	1.66	1.54
2	B	376	GLU	CG-CD	5.73	1.60	1.51
1	G	34	GLU	CB-CG	5.73	1.63	1.52
1	K	183	TYR	CD2-CE2	5.73	1.48	1.39
2	F	396	LEU	C-O	5.73	1.34	1.23
1	G	188	ARG	NE-CZ	5.73	1.40	1.33
2	L	314	ASN	C-O	-5.72	1.12	1.23
2	H	402	ALA	CA-CB	5.72	1.64	1.52
1	E	71	TRP	CZ2-CH2	5.72	1.48	1.37
2	D	388	TYR	CD1-CE1	5.71	1.48	1.39
1	I	150	GLN	CB-CG	5.71	1.68	1.52
1	K	146	ASP	C-O	5.71	1.34	1.23
1	C	151	ALA	CA-CB	5.71	1.64	1.52
2	B	383	ARG	CB-CG	-5.71	1.37	1.52
2	B	523	PHE	CD1-CE1	-5.71	1.27	1.39
2	B	326	THR	N-CA	5.70	1.57	1.46
2	J	321	THR	CB-CG2	5.70	1.71	1.52
2	J	392	VAL	CB-CG1	-5.70	1.40	1.52
1	K	157	VAL	CB-CG1	5.70	1.64	1.52
1	I	157	VAL	CB-CG2	-5.70	1.40	1.52
2	D	318	LYS	C-O	5.69	1.34	1.23
2	J	305	ASN	CB-CG	5.69	1.64	1.51
2	L	519	LEU	CA-CB	5.68	1.66	1.53
2	J	522	ARG	CZ-NH2	5.68	1.40	1.33
1	K	42	PRO	N-CA	5.68	1.56	1.47
2	H	447	TYR	CD1-CE1	5.68	1.47	1.39
2	F	333	ARG	CG-CD	5.67	1.66	1.51
1	G	9	PRO	CB-CG	-5.67	1.21	1.50
1	C	101	ALA	C-N	5.67	1.43	1.33
2	J	437	TYR	C-O	5.67	1.34	1.23
2	F	481	GLU	CB-CG	-5.66	1.41	1.52
2	L	450	ARG	CZ-NH1	5.66	1.40	1.33
1	C	180	LYS	CD-CE	5.66	1.65	1.51
2	D	378	ILE	CA-CB	5.66	1.67	1.54
2	B	436	TYR	CB-CG	-5.66	1.43	1.51
1	K	42	PRO	CB-CG	5.66	1.78	1.50
2	L	411	LYS	CD-CE	5.64	1.65	1.51
2	D	503	GLN	CA-CB	-5.64	1.41	1.53
2	H	439	PHE	CD1-CE1	5.64	1.50	1.39
1	A	176	GLU	CG-CD	5.64	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	501	VAL	CB-CG1	-5.64	1.41	1.52
1	C	197	PHE	CE2-CZ	5.63	1.48	1.37
1	E	56	TYR	CZ-OH	5.63	1.47	1.37
1	G	194	GLU	CG-CD	5.63	1.60	1.51
2	F	387	GLN	C-O	-5.63	1.12	1.23
2	H	411	LYS	CD-CE	5.63	1.65	1.51
1	E	197	PHE	CD2-CE2	5.63	1.50	1.39
2	D	404	ALA	CA-CB	5.62	1.64	1.52
2	J	330	ARG	CZ-NH2	5.62	1.40	1.33
1	C	24	GLU	CB-CG	5.62	1.62	1.52
2	H	411	LYS	CE-NZ	5.62	1.63	1.49
1	A	200	PHE	CG-CD1	5.61	1.47	1.38
2	D	345	GLU	CB-CG	-5.61	1.41	1.52
1	G	113	VAL	CB-CG1	-5.61	1.41	1.52
2	H	346	THR	CA-CB	-5.61	1.38	1.53
2	J	315	TRP	CG-CD1	-5.61	1.28	1.36
1	C	89	PHE	CE2-CZ	5.61	1.48	1.37
2	D	306	SER	C-O	-5.61	1.12	1.23
1	I	104	TRP	C-O	5.60	1.33	1.23
2	J	439	PHE	CE1-CZ	5.60	1.48	1.37
1	K	111	PRO	C-O	5.60	1.34	1.23
1	G	103	GLU	CB-CG	-5.60	1.41	1.52
1	C	117	ALA	CA-CB	-5.60	1.40	1.52
1	C	36	TRP	CB-CG	-5.59	1.40	1.50
2	D	473	LYS	CE-NZ	5.58	1.63	1.49
1	A	197	PHE	CG-CD1	5.58	1.47	1.38
1	A	197	PHE	CG-CD2	5.58	1.47	1.38
2	L	395	THR	C-O	5.58	1.33	1.23
2	H	389	GLY	C-O	-5.58	1.14	1.23
1	K	38	ARG	CG-CD	5.57	1.65	1.51
1	K	79	TYR	CD2-CE2	5.57	1.47	1.39
1	G	99	PHE	CG-CD2	5.57	1.47	1.38
2	F	456	TRP	CG-CD1	5.56	1.44	1.36
2	B	463	PHE	CE2-CZ	-5.56	1.26	1.37
2	H	409	ARG	CB-CG	-5.56	1.37	1.52
1	I	97	THR	C-O	5.56	1.33	1.23
2	J	308	PHE	C-O	5.56	1.33	1.23
2	D	305	ASN	CB-CG	5.55	1.63	1.51
2	F	417	ALA	C-O	5.55	1.33	1.23
2	L	351	PHE	C-O	5.55	1.33	1.23
1	G	173	LYS	CA-CB	5.55	1.66	1.53
1	K	99	PHE	CD2-CE2	5.55	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	492	VAL	CB-CG1	5.55	1.64	1.52
1	G	130	LEU	CG-CD2	5.55	1.72	1.51
2	H	523	PHE	CE2-CZ	-5.55	1.26	1.37
1	I	68	LEU	CG-CD2	-5.55	1.31	1.51
2	J	520	ALA	C-O	5.55	1.33	1.23
1	C	7	GLU	CB-CG	5.54	1.62	1.52
1	A	119	GLY	C-O	5.54	1.32	1.23
2	D	324	TYR	CD1-CE1	5.54	1.47	1.39
2	D	507	LYS	CD-CE	5.54	1.65	1.51
1	A	7	GLU	CD-OE2	5.54	1.31	1.25
2	F	438	SER	CA-CB	-5.54	1.44	1.52
2	H	356	PHE	CB-CG	-5.54	1.42	1.51
2	J	450	ARG	CZ-NH2	5.54	1.40	1.33
1	K	79	TYR	CD1-CE1	5.54	1.47	1.39
2	B	483	ASP	CB-CG	-5.53	1.40	1.51
2	F	377	ARG	CB-CG	5.53	1.67	1.52
1	K	194	GLU	CD-OE2	-5.53	1.19	1.25
1	G	188	ARG	CZ-NH2	5.53	1.40	1.33
2	B	330	ARG	CG-CD	-5.53	1.38	1.51
2	B	521	TYR	CD1-CE1	-5.53	1.31	1.39
2	J	437	TYR	CZ-OH	5.53	1.47	1.37
1	E	114	VAL	CB-CG1	5.52	1.64	1.52
1	I	62	LEU	C-O	5.52	1.33	1.23
2	L	530	GLN	N-CA	5.52	1.57	1.46
1	C	150	GLN	CD-OE1	5.52	1.36	1.24
1	E	2	ILE	CG1-CD1	-5.52	1.12	1.50
2	J	447	TYR	CG-CD1	5.52	1.46	1.39
2	L	306	SER	CB-OG	-5.52	1.35	1.42
1	G	24	GLU	CB-CG	5.51	1.62	1.52
2	L	398	GLU	CB-CG	-5.51	1.41	1.52
2	F	493	LYS	CD-CE	5.50	1.65	1.51
1	A	188	ARG	CZ-NH1	5.50	1.40	1.33
1	A	7	GLU	CD-OE1	5.50	1.31	1.25
2	J	436	TYR	CG-CD1	5.50	1.46	1.39
1	K	178	ASP	CB-CG	5.50	1.63	1.51
2	D	423	PHE	CB-CG	-5.50	1.42	1.51
2	F	367	PHE	CG-CD1	5.49	1.47	1.38
2	L	390	LYS	CG-CD	5.49	1.71	1.52
1	E	35	ILE	CA-CB	-5.49	1.42	1.54
2	F	331	SER	CB-OG	5.49	1.49	1.42
1	G	131	PHE	CD2-CE2	5.48	1.50	1.39
1	K	131	PHE	CG-CD2	5.48	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	412	ASN	CB-CG	5.48	1.63	1.51
2	D	414	ARG	CZ-NH2	5.48	1.40	1.33
2	B	428	ARG	CG-CD	-5.48	1.38	1.51
1	E	131	PHE	CE2-CZ	5.48	1.47	1.37
2	J	403	ASN	C-O	5.48	1.33	1.23
2	J	506	ALA	CA-CB	-5.47	1.41	1.52
2	F	447	TYR	CB-CG	-5.47	1.43	1.51
2	J	491	ILE	N-CA	5.47	1.57	1.46
1	K	154	LYS	CD-CE	5.46	1.65	1.51
1	C	150	GLN	CG-CD	5.46	1.63	1.51
2	J	396	LEU	C-O	5.46	1.33	1.23
1	C	103	GLU	CG-CD	5.46	1.60	1.51
1	A	78	GLU	CG-CD	5.45	1.60	1.51
2	J	314	ASN	CB-CG	5.45	1.63	1.51
1	A	168	GLU	CD-OE2	5.45	1.31	1.25
2	B	453	PRO	CB-CG	5.45	1.77	1.50
2	D	479	TYR	CD1-CE1	-5.44	1.31	1.39
1	I	107	HIS	C-O	5.44	1.33	1.23
2	B	452	GLY	C-O	5.44	1.32	1.23
1	E	200	PHE	CE2-CZ	5.44	1.47	1.37
2	F	358	ALA	CA-CB	5.44	1.63	1.52
1	A	176	GLU	CD-OE1	5.44	1.31	1.25
2	L	376	GLU	CD-OE2	5.44	1.31	1.25
1	E	198	PHE	CE2-CZ	5.43	1.47	1.37
2	B	528	ARG	CB-CG	5.42	1.67	1.52
1	C	16	TYR	CD2-CE2	5.42	1.47	1.39
2	L	315	TRP	CE3-CZ3	5.42	1.47	1.38
2	D	516	MET	CB-CG	5.42	1.68	1.51
2	B	310	ILE	CB-CG2	5.42	1.69	1.52
1	E	17	VAL	CB-CG1	5.41	1.64	1.52
2	F	317	PRO	CA-C	5.41	1.63	1.52
1	G	91	SER	CA-CB	-5.41	1.44	1.52
1	K	36	TRP	CZ3-CH2	5.41	1.48	1.40
2	H	402	ALA	C-O	5.40	1.33	1.23
1	K	133	ARG	CB-CG	-5.40	1.38	1.52
1	A	99	PHE	CD1-CE1	5.40	1.50	1.39
1	K	151	ALA	C-O	5.40	1.33	1.23
2	D	482	GLY	C-O	-5.39	1.15	1.23
1	K	99	PHE	CE1-CZ	5.39	1.47	1.37
1	E	80	GLN	CB-CG	5.39	1.67	1.52
2	D	440	ARG	CZ-NH2	-5.39	1.26	1.33
1	K	174	ARG	CZ-NH2	5.39	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	99	PHE	CD1-CE1	5.39	1.50	1.39
1	G	47	GLU	CB-CG	-5.39	1.42	1.52
2	B	466	SER	CB-OG	5.39	1.49	1.42
1	E	188	ARG	CD-NE	5.39	1.55	1.46
1	E	71	TRP	CD2-CE2	5.38	1.47	1.41
1	E	104	TRP	CE3-CZ3	5.38	1.47	1.38
2	F	537	ASN	N-CA	5.38	1.57	1.46
2	H	426	VAL	CA-CB	-5.38	1.43	1.54
1	G	161	ILE	CB-CG2	5.38	1.69	1.52
2	L	477	GLN	C-O	5.38	1.33	1.23
2	B	428	ARG	CB-CG	-5.38	1.38	1.52
1	A	187	ILE	CB-CG2	5.38	1.69	1.52
1	A	86	GLU	CB-CG	5.38	1.62	1.52
2	D	513	ALA	N-CA	-5.38	1.35	1.46
2	L	329	ALA	CA-CB	-5.37	1.41	1.52
2	D	450	ARG	CZ-NH2	5.37	1.40	1.33
1	K	16	TYR	CE2-CZ	5.37	1.45	1.38
1	E	38	ARG	CG-CD	5.37	1.65	1.51
2	H	467	GLY	N-CA	-5.37	1.38	1.46
2	H	381	ALA	CA-CB	-5.37	1.41	1.52
2	L	440	ARG	CZ-NH1	5.37	1.40	1.33
1	E	69	GLU	CG-CD	5.36	1.59	1.51
1	G	168	GLU	CB-CG	5.36	1.62	1.52
2	D	537	ASN	N-CA	5.36	1.57	1.46
1	K	92	PHE	CG-CD2	5.36	1.46	1.38
2	B	521	TYR	CG-CD2	5.35	1.46	1.39
1	C	200	PHE	CE2-CZ	5.35	1.47	1.37
1	I	176	GLU	CD-OE2	5.35	1.31	1.25
1	C	166	ARG	CD-NE	-5.35	1.37	1.46
1	E	80	GLN	CG-CD	5.35	1.63	1.51
2	F	449	TRP	CE3-CZ3	5.35	1.47	1.38
2	J	335	ALA	CA-CB	5.35	1.63	1.52
1	A	183	TYR	CE2-CZ	-5.35	1.31	1.38
2	H	324	TYR	CZ-OH	-5.35	1.28	1.37
1	G	198	PHE	CB-CG	-5.34	1.42	1.51
2	L	318	LYS	CB-CG	-5.34	1.38	1.52
1	K	16	TYR	CE1-CZ	5.34	1.45	1.38
2	F	450	ARG	NE-CZ	5.34	1.40	1.33
2	D	415	TYR	CD2-CE2	-5.34	1.31	1.39
2	L	377	ARG	CG-CD	5.34	1.65	1.51
2	B	521	TYR	CE1-CZ	5.33	1.45	1.38
1	G	197	PHE	CD1-CE1	5.33	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	332	PRO	C-O	5.33	1.33	1.23
1	I	189	ILE	CA-CB	-5.33	1.42	1.54
1	I	56	TYR	CZ-OH	5.33	1.47	1.37
1	A	138	HIS	C-O	-5.33	1.13	1.23
1	G	196	VAL	CB-CG1	5.33	1.64	1.52
2	J	388	TYR	CG-CD2	5.33	1.46	1.39
1	E	180	LYS	CE-NZ	5.32	1.62	1.49
1	G	114	VAL	CA-CB	5.32	1.66	1.54
1	E	188	ARG	CZ-NH1	5.32	1.40	1.33
1	G	165	GLN	CD-NE2	5.32	1.46	1.32
1	A	3	GLU	CD-OE1	5.32	1.31	1.25
1	E	13	ALA	N-CA	5.31	1.56	1.46
2	F	522	ARG	C-O	5.31	1.33	1.23
2	J	415	TYR	CD2-CE2	-5.31	1.31	1.39
2	J	499	GLU	CD-OE2	5.31	1.31	1.25
1	K	108	THR	CA-CB	5.31	1.67	1.53
2	J	324	TYR	CG-CD1	5.30	1.46	1.39
1	C	200	PHE	C-OXT	5.30	1.33	1.23
1	K	63	VAL	CB-CG2	-5.30	1.41	1.52
2	H	460	HIS	CA-CB	-5.30	1.42	1.53
1	I	131	PHE	CG-CD2	5.30	1.46	1.38
2	D	469	SER	C-O	-5.30	1.13	1.23
2	J	401	GLN	CD-NE2	5.30	1.46	1.32
2	D	521	TYR	CD1-CE1	5.30	1.47	1.39
2	F	437	TYR	CB-CG	5.30	1.59	1.51
2	F	481	GLU	CD-OE2	-5.29	1.19	1.25
2	F	448	PRO	CA-C	-5.29	1.42	1.52
1	I	178	ASP	CB-CG	5.29	1.62	1.51
1	K	150	GLN	CG-CD	5.29	1.63	1.51
2	B	383	ARG	C-O	5.29	1.33	1.23
1	E	72	GLN	CD-OE1	5.29	1.35	1.24
1	E	97	THR	CB-CG2	-5.29	1.34	1.52
2	B	312	ASP	CB-CG	5.29	1.62	1.51
1	G	71	TRP	CD2-CE2	5.29	1.47	1.41
2	F	428	ARG	CB-CG	-5.29	1.38	1.52
2	F	394	ASN	C-O	-5.28	1.13	1.23
1	I	17	VAL	CA-CB	-5.28	1.43	1.54
1	K	112	GLY	C-O	-5.28	1.15	1.23
1	A	56	TYR	CE1-CZ	5.28	1.45	1.38
1	C	55	VAL	CB-CG1	-5.28	1.41	1.52
1	C	16	TYR	CB-CG	5.27	1.59	1.51
1	C	35	ILE	CA-CB	-5.27	1.42	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	502	GLN	CD-NE2	5.26	1.46	1.32
2	J	368	ASN	CA-CB	5.26	1.66	1.53
1	A	116	ASN	C-O	5.26	1.33	1.23
1	C	38	ARG	CZ-NH2	5.26	1.39	1.33
2	B	490	PRO	CG-CD	-5.26	1.33	1.50
1	K	43	ASP	C-O	5.26	1.33	1.23
2	H	351	PHE	CE2-CZ	5.26	1.47	1.37
1	C	86	GLU	CD-OE1	5.25	1.31	1.25
2	H	318	LYS	CE-NZ	5.25	1.62	1.49
2	H	475	ILE	C-O	5.25	1.33	1.23
1	K	184	ARG	CG-CD	5.25	1.65	1.51
1	A	41	LYS	CE-NZ	5.24	1.62	1.49
2	D	532	LYS	CA-CB	5.24	1.65	1.53
1	G	97	THR	CB-CG2	-5.24	1.35	1.52
1	K	150	GLN	CD-OE1	5.24	1.35	1.24
1	K	185	PHE	CD2-CE2	5.24	1.49	1.39
2	B	311	ARG	C-O	5.23	1.33	1.23
1	C	198	PHE	CE2-CZ	5.23	1.47	1.37
2	D	515	PRO	CB-CG	5.23	1.76	1.50
1	G	89	PHE	CD2-CE2	5.23	1.49	1.39
2	B	462	HIS	C-O	-5.23	1.13	1.23
2	H	318	LYS	CB-CG	5.23	1.66	1.52
1	K	34	GLU	CB-CG	-5.23	1.42	1.52
2	B	537	ASN	CG-OD1	5.22	1.35	1.24
2	D	388	TYR	CG-CD2	5.22	1.46	1.39
2	L	319	ALA	CA-CB	-5.22	1.41	1.52
1	A	188	ARG	CG-CD	5.22	1.65	1.51
2	B	335	ALA	CA-C	5.22	1.66	1.52
1	C	7	GLU	C-O	5.21	1.33	1.23
2	B	388	TYR	CG-CD1	5.21	1.46	1.39
2	D	415	TYR	CG-CD2	5.21	1.46	1.39
2	F	460	HIS	CA-C	-5.21	1.39	1.52
2	H	514	ASN	CG-OD1	5.21	1.35	1.24
1	I	138	HIS	C-O	-5.21	1.13	1.23
2	F	414	ARG	CZ-NH2	5.21	1.39	1.33
1	K	100	ASP	CB-CG	5.20	1.62	1.51
2	J	317	PRO	CB-CG	5.20	1.75	1.50
2	J	310	ILE	N-CA	-5.20	1.35	1.46
2	J	368	ASN	N-CA	5.20	1.56	1.46
1	K	78	GLU	CG-CD	5.20	1.59	1.51
1	A	94	ARG	CD-NE	-5.19	1.37	1.46
1	K	79	TYR	CE2-CZ	-5.19	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	163	GLN	CD-NE2	5.19	1.45	1.32
1	G	178	ASP	CB-CG	5.19	1.62	1.51
2	D	380	VAL	CB-CG2	-5.18	1.42	1.52
2	F	314	ASN	CG-OD1	5.18	1.35	1.24
1	C	97	THR	CB-CG2	-5.18	1.35	1.52
2	F	535	PHE	CE1-CZ	5.18	1.47	1.37
2	B	313	ARG	CZ-NH2	-5.18	1.26	1.33
1	G	78	GLU	CD-OE1	5.17	1.31	1.25
1	A	154	LYS	CG-CD	5.17	1.70	1.52
1	E	197	PHE	CG-CD1	5.17	1.46	1.38
1	K	80	GLN	CG-CD	5.17	1.62	1.51
2	J	522	ARG	C-O	5.17	1.33	1.23
2	L	535	PHE	CG-CD2	5.17	1.46	1.38
2	F	449	TRP	CD2-CE2	5.16	1.47	1.41
2	L	480	PHE	CG-CD2	5.16	1.46	1.38
1	A	83	TYR	CE2-CZ	5.16	1.45	1.38
2	J	308	PHE	CE1-CZ	-5.15	1.27	1.37
2	D	337	VAL	C-O	5.15	1.33	1.23
2	B	414	ARG	NE-CZ	5.15	1.39	1.33
1	E	101	ALA	CA-CB	5.14	1.63	1.52
2	J	311	ARG	N-CA	-5.14	1.36	1.46
2	B	318	LYS	CE-NZ	5.14	1.61	1.49
2	B	439	PHE	CG-CD1	5.14	1.46	1.38
2	L	537	ASN	N-CA	5.14	1.56	1.46
2	B	449	TRP	CB-CG	-5.14	1.41	1.50
2	F	388	TYR	CB-CG	5.13	1.59	1.51
1	I	6	PRO	CA-C	5.13	1.63	1.52
1	C	165	GLN	CG-CD	5.13	1.62	1.51
1	E	138	HIS	N-CA	-5.13	1.36	1.46
2	J	330	ARG	CG-CD	-5.13	1.39	1.51
2	F	344	SER	C-O	-5.12	1.13	1.23
1	C	64	ARG	CG-CD	-5.12	1.39	1.51
2	B	406	GLY	C-O	5.11	1.31	1.23
2	D	390	LYS	CG-CD	5.11	1.69	1.52
2	D	442	ILE	C-O	-5.11	1.13	1.23
2	H	445	GLY	C-O	5.11	1.31	1.23
2	D	503	GLN	CD-OE1	5.11	1.35	1.24
2	F	370	GLY	C-O	5.11	1.31	1.23
2	J	516	MET	CG-SD	5.11	1.94	1.81
1	I	71	TRP	CE3-CZ3	5.11	1.47	1.38
1	C	110	LYS	CB-CG	-5.10	1.38	1.52
2	L	436	TYR	CG-CD2	5.10	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	521	TYR	CE2-CZ	5.10	1.45	1.38
2	H	374	ILE	CA-C	5.10	1.66	1.52
1	I	91	SER	CA-CB	-5.10	1.45	1.52
1	A	190	GLN	C-O	-5.10	1.13	1.23
2	D	325	LYS	CD-CE	5.10	1.64	1.51
2	B	536	GLU	CD-OE2	-5.09	1.20	1.25
2	F	381	ALA	CA-CB	-5.09	1.41	1.52
1	I	144	TYR	CG-CD1	5.09	1.45	1.39
1	K	176	GLU	CD-OE1	5.09	1.31	1.25
2	B	327	SER	CB-OG	-5.09	1.35	1.42
1	E	41	LYS	CE-NZ	5.08	1.61	1.49
2	J	408[A]	CYS	CB-SG	5.08	1.90	1.82
2	J	408[B]	CYS	CB-SG	5.08	1.90	1.82
1	C	145	PHE	CE1-CZ	5.08	1.47	1.37
2	D	389	GLY	C-O	-5.08	1.15	1.23
2	F	319	ALA	CA-CB	5.08	1.63	1.52
1	E	116	ASN	C-O	5.07	1.32	1.23
2	B	435	GLY	C-O	5.07	1.31	1.23
1	C	174	ARG	CZ-NH2	5.06	1.39	1.33
2	J	407	ARG	CZ-NH2	5.06	1.39	1.33
2	D	537	ASN	CB-CG	5.06	1.62	1.51
1	G	100	ASP	N-CA	5.06	1.56	1.46
1	K	154	LYS	CE-NZ	5.06	1.61	1.49
2	H	382	GLY	C-O	-5.05	1.15	1.23
2	B	313	ARG	CZ-NH1	5.05	1.39	1.33
2	D	476	THR	CB-CG2	-5.05	1.35	1.52
2	J	476	THR	N-CA	-5.05	1.36	1.46
2	L	439	PHE	CD2-CE2	5.05	1.49	1.39
1	C	91	SER	CA-CB	-5.04	1.45	1.52
2	D	475	ILE	CB-CG2	5.03	1.68	1.52
1	E	63	VAL	CB-CG2	-5.03	1.42	1.52
2	H	450	ARG	CG-CD	5.03	1.64	1.51
2	H	481	GLU	C-O	5.03	1.32	1.23
1	A	168	GLU	CG-CD	5.03	1.59	1.51
1	C	119	GLY	N-CA	5.03	1.53	1.46
2	B	447	TYR	CB-CG	-5.03	1.44	1.51
2	B	344	SER	CB-OG	-5.02	1.35	1.42
1	I	89	PHE	C-O	5.02	1.32	1.23
2	L	535	PHE	CE1-CZ	5.02	1.46	1.37
1	A	139	LEU	CG-CD2	5.02	1.70	1.51
2	D	380	VAL	CB-CG1	-5.02	1.42	1.52
2	D	501	VAL	C-O	-5.02	1.13	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	174	ARG	CB-CG	-5.02	1.39	1.52
2	B	301	PRO	CG-CD	5.01	1.67	1.50
2	B	436	TYR	CD2-CE2	5.01	1.46	1.39
1	G	37	ASN	CG-OD1	-5.01	1.12	1.24
1	G	104	TRP	CB-CG	-5.01	1.41	1.50
1	K	76	ASN	CB-CG	5.01	1.62	1.51
1	C	103	GLU	CD-OE1	5.00	1.31	1.25
1	E	165	GLN	CG-CD	5.00	1.62	1.51
2	H	493	LYS	CD-CE	5.00	1.63	1.51
2	B	526	VAL	N-CA	-5.00	1.36	1.46
1	E	183	TYR	CG-CD2	5.00	1.45	1.39
1	A	109	VAL	CB-CG2	-5.00	1.42	1.52
2	B	303	GLN	CA-C	5.00	1.66	1.52

All (532) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	440	ARG	NE-CZ-NH2	-25.00	107.80	120.30
2	D	440	ARG	NE-CZ-NH1	23.66	132.13	120.30
2	B	440	ARG	NE-CZ-NH2	-21.69	109.45	120.30
2	F	440	ARG	NE-CZ-NH2	-21.17	109.72	120.30
1	G	94	ARG	NE-CZ-NH2	-20.84	109.88	120.30
1	G	94	ARG	NE-CZ-NH1	20.10	130.35	120.30
2	H	440	ARG	NE-CZ-NH1	19.21	129.91	120.30
2	H	440	ARG	NE-CZ-NH2	-18.78	110.91	120.30
2	D	333	ARG	NE-CZ-NH1	-18.11	111.25	120.30
2	L	440	ARG	NE-CZ-NH2	-17.53	111.53	120.30
2	L	428	ARG	NE-CZ-NH2	-16.85	111.87	120.30
1	K	94	ARG	NE-CZ-NH2	-15.66	112.47	120.30
1	A	94	ARG	NE-CZ-NH2	-15.26	112.67	120.30
1	A	94	ARG	NE-CZ-NH1	14.97	127.78	120.30
1	C	184	ARG	NE-CZ-NH2	-14.53	113.03	120.30
1	C	188	ARG	NE-CZ-NH2	-14.49	113.05	120.30
2	B	330	ARG	NE-CZ-NH2	-14.30	113.15	120.30
2	H	538	CYS	CA-CB-SG	-13.97	88.86	114.00
1	E	81	ASP	CB-CG-OD1	13.85	130.76	118.30
2	J	440	ARG	NE-CZ-NH2	-13.84	113.38	120.30
2	B	538	CYS	CA-CB-SG	-13.70	89.33	114.00
1	E	184	ARG	NE-CZ-NH2	-13.69	113.46	120.30
1	I	142	ARG	NE-CZ-NH2	-13.50	113.55	120.30
1	I	142	ARG	NE-CZ-NH1	13.21	126.91	120.30
1	A	38	ARG	NE-CZ-NH2	-13.17	113.72	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	440	ARG	NE-CZ-NH1	13.05	126.83	120.30
1	K	133	ARG	NE-CZ-NH2	-12.98	113.81	120.30
1	C	64	ARG	NE-CZ-NH2	-12.95	113.83	120.30
1	E	65	ASP	CB-CG-OD1	12.77	129.79	118.30
2	D	428	ARG	NE-CZ-NH2	-12.73	113.94	120.30
2	F	428	ARG	NE-CZ-NH2	-12.73	113.94	120.30
2	F	330	ARG	NE-CZ-NH2	-12.49	114.05	120.30
1	K	94	ARG	NE-CZ-NH1	12.31	126.45	120.30
1	C	106	LEU	CB-CG-CD2	-12.22	90.22	111.00
2	H	450	ARG	NE-CZ-NH1	-12.21	114.20	120.30
2	F	457	ARG	NE-CZ-NH2	-12.16	114.22	120.30
2	J	377	ARG	NE-CZ-NH1	-12.12	114.24	120.30
1	C	188	ARG	NE-CZ-NH1	12.11	126.36	120.30
2	F	440	ARG	NE-CZ-NH1	12.05	126.33	120.30
2	H	428	ARG	NE-CZ-NH2	-11.50	114.55	120.30
2	B	531	ARG	NE-CZ-NH1	-11.47	114.57	120.30
2	D	510	MET	CG-SD-CE	-11.27	82.17	100.20
1	E	81	ASP	CB-CG-OD2	-11.26	108.17	118.30
1	I	166	ARG	NE-CZ-NH1	11.02	125.81	120.30
2	F	428	ARG	NE-CZ-NH1	11.02	125.81	120.30
2	H	330	ARG	NE-CZ-NH1	-10.97	114.81	120.30
2	L	414	ARG	NE-CZ-NH1	10.84	125.72	120.30
2	D	440	ARG	CB-CG-CD	-10.78	83.58	111.60
2	H	428	ARG	NE-CZ-NH1	10.74	125.67	120.30
1	C	133	ARG	NE-CZ-NH1	10.68	125.64	120.30
2	J	447	TYR	CB-CG-CD2	-10.64	114.62	121.00
1	G	184	ARG	NE-CZ-NH2	-10.63	114.99	120.30
1	I	189	ILE	CG1-CB-CG2	-10.56	88.18	111.40
2	D	473	LYS	CD-CE-NZ	-10.48	87.60	111.70
1	K	106	LEU	CB-CG-CD2	-10.46	93.21	111.00
2	J	504	LEU	CB-CG-CD1	-10.45	93.23	111.00
2	F	528	ARG	NE-CZ-NH2	-10.39	115.11	120.30
2	B	447	TYR	CB-CG-CD2	-10.27	114.84	121.00
1	K	52	LEU	CA-CB-CG	10.19	138.74	115.30
2	B	528	ARG	NE-CZ-NH1	-10.19	115.20	120.30
2	J	416	LEU	CA-CB-CG	10.11	138.54	115.30
2	L	333	ARG	NE-CZ-NH1	10.05	125.33	120.30
1	E	52	LEU	CA-CB-CG	10.04	138.38	115.30
1	E	188	ARG	NE-CZ-NH1	10.02	125.31	120.30
1	G	184	ARG	NE-CZ-NH1	10.02	125.31	120.30
2	F	311	ARG	NE-CZ-NH2	-9.86	115.37	120.30
2	B	440	ARG	NE-CZ-NH1	9.86	125.23	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	428	ARG	NE-CZ-NH1	9.85	125.22	120.30
1	C	166	ARG	NE-CZ-NH1	9.84	125.22	120.30
2	H	524	ASP	CB-CG-OD1	9.83	127.14	118.30
1	C	167	ARG	NE-CZ-NH1	-9.81	115.39	120.30
1	E	106	LEU	CB-CG-CD2	-9.80	94.34	111.00
2	L	528	ARG	NE-CZ-NH1	-9.80	115.40	120.30
2	L	538	CYS	CA-CB-SG	-9.78	96.39	114.00
1	I	64	ARG	NE-CZ-NH1	9.77	125.18	120.30
2	B	420	ASP	CB-CG-OD2	-9.76	109.52	118.30
1	I	94	ARG	NE-CZ-NH1	9.73	125.17	120.30
2	B	522	ARG	NE-CZ-NH1	-9.71	115.44	120.30
1	K	38	ARG	NE-CZ-NH2	-9.71	115.44	120.30
1	A	52	LEU	CA-CB-CG	9.71	137.63	115.30
2	H	377	ARG	NE-CZ-NH1	-9.65	115.47	120.30
1	G	65	ASP	CB-CG-OD2	-9.60	109.66	118.30
2	J	360	ASP	CB-CG-OD2	-9.56	109.69	118.30
1	K	31	ARG	NE-CZ-NH1	-9.56	115.52	120.30
1	A	74	ASP	CB-CG-OD2	-9.53	109.72	118.30
1	E	64	ARG	NE-CZ-NH2	-9.51	115.55	120.30
2	J	522	ARG	NE-CZ-NH1	-9.48	115.56	120.30
1	E	139	LEU	CB-CG-CD1	-9.45	94.94	111.00
1	I	133	ARG	NE-CZ-NH1	9.42	125.01	120.30
2	D	339	ILE	CG1-CB-CG2	-9.36	90.80	111.40
2	F	474	LEU	CB-CG-CD2	-9.31	95.17	111.00
2	L	447	TYR	CB-CG-CD2	-9.30	115.42	121.00
1	I	184	ARG	NE-CZ-NH2	-9.30	115.65	120.30
1	A	188	ARG	NE-CZ-NH1	9.28	124.94	120.30
2	J	473	LYS	CD-CE-NZ	-9.27	90.38	111.70
1	E	52	LEU	CB-CG-CD2	-9.26	95.26	111.00
1	A	175	CYS	CA-CB-SG	9.24	130.63	114.00
2	J	330	ARG	NE-CZ-NH2	-9.23	115.68	120.30
2	H	409	ARG	NE-CZ-NH1	9.16	124.88	120.30
2	J	409	ARG	NE-CZ-NH1	9.12	124.86	120.30
1	A	74	ASP	CB-CG-OD1	9.05	126.45	118.30
2	B	495	ILE	CG1-CB-CG2	-9.03	91.54	111.40
1	A	188	ARG	NE-CZ-NH2	-9.00	115.80	120.30
2	D	434	ASP	CB-CG-OD1	-8.99	110.21	118.30
2	J	414	ARG	NE-CZ-NH1	8.89	124.74	120.30
2	H	330	ARG	NE-CZ-NH2	8.88	124.74	120.30
1	C	174	ARG	NE-CZ-NH1	-8.86	115.87	120.30
2	D	531	ARG	NE-CZ-NH2	-8.75	115.92	120.30
2	F	531	ARG	NE-CZ-NH2	-8.70	115.95	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	65	ASP	CB-CG-OD1	8.64	126.08	118.30
2	D	409	ARG	NE-CZ-NH2	-8.52	116.04	120.30
2	J	493	LYS	CD-CE-NZ	8.52	131.29	111.70
2	B	330	ARG	NE-CZ-NH1	8.49	124.54	120.30
1	A	32	ASP	CB-CG-OD2	-8.46	110.68	118.30
2	L	333	ARG	NE-CZ-NH2	-8.46	116.07	120.30
1	I	94	ARG	NE-CZ-NH2	-8.45	116.07	120.30
2	L	440	ARG	NE-CZ-NH1	8.44	124.52	120.30
1	C	32	ASP	CB-CG-OD1	-8.44	110.70	118.30
2	D	538	CYS	CA-CB-SG	-8.41	98.86	114.00
2	J	336	LEU	CB-CG-CD2	-8.40	96.71	111.00
2	H	473	LYS	CD-CE-NZ	-8.38	92.42	111.70
1	A	39	LEU	CB-CG-CD2	-8.38	96.76	111.00
1	K	133	ARG	NE-CZ-NH1	8.36	124.48	120.30
2	J	508	LEU	CB-CG-CD2	-8.35	96.81	111.00
1	A	199	ASP	CB-CG-OD2	8.33	125.79	118.30
2	B	413	ASP	CB-CG-OD2	-8.31	110.82	118.30
2	D	333	ARG	NE-CZ-NH2	8.27	124.44	120.30
1	I	188	ARG	NE-CZ-NH1	8.27	124.43	120.30
2	B	440	ARG	CB-CG-CD	-8.24	90.17	111.60
1	C	158	LEU	CA-CB-CG	8.22	134.20	115.30
2	L	428	ARG	NE-CZ-NH1	8.18	124.39	120.30
2	F	440	ARG	CB-CG-CD	-8.15	90.42	111.60
1	G	38	ARG	NE-CZ-NH2	-8.14	116.23	120.30
2	J	428	ARG	NE-CZ-NH2	-8.14	116.23	120.30
2	B	313	ARG	NE-CZ-NH1	8.14	124.37	120.30
1	I	2	ILE	CG1-CB-CG2	-8.11	93.55	111.40
2	L	388	TYR	CB-CG-CD1	-8.06	116.16	121.00
1	K	167	ARG	NE-CZ-NH2	8.05	124.33	120.30
1	C	31	ARG	NE-CZ-NH2	8.02	124.31	120.30
1	K	31	ARG	NE-CZ-NH2	8.02	124.31	120.30
2	D	483	ASP	CB-CG-OD2	7.98	125.48	118.30
1	E	38	ARG	NE-CZ-NH1	7.96	124.28	120.30
1	C	186	ASP	CB-CG-OD1	7.95	125.46	118.30
2	F	311	ARG	NE-CZ-NH1	7.95	124.28	120.30
1	G	175	CYS	CA-CB-SG	7.95	128.31	114.00
2	J	304	ASP	CB-CG-OD1	7.91	125.42	118.30
2	D	386	ASP	CB-CG-OD1	-7.91	111.18	118.30
1	C	94	ARG	NE-CZ-NH1	7.86	124.23	120.30
1	A	174	ARG	NE-CZ-NH2	-7.85	116.37	120.30
2	F	517	ASP	CB-CG-OD2	-7.84	111.24	118.30
1	A	178	ASP	CB-CG-OD2	7.84	125.35	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	188	ARG	NE-CZ-NH1	7.82	124.21	120.30
2	H	365	LEU	CB-CG-CD1	-7.81	97.72	111.00
2	B	428	ARG	NE-CZ-NH2	-7.81	116.40	120.30
2	F	434	ASP	CB-CG-OD1	-7.79	111.29	118.30
2	H	475	ILE	CA-CB-CG1	7.78	125.78	111.00
1	I	94	ARG	CB-CG-CD	7.78	131.82	111.60
2	B	428	ARG	NE-CZ-NH1	7.76	124.18	120.30
2	H	437	TYR	CZ-CE2-CD2	7.75	126.77	119.80
2	F	442	ILE	CG1-CB-CG2	-7.74	94.38	111.40
1	K	39	LEU	CB-CG-CD2	-7.73	97.85	111.00
2	F	447	TYR	CB-CG-CD2	-7.71	116.37	121.00
2	D	414	ARG	NE-CZ-NH2	-7.70	116.45	120.30
2	L	383	ARG	NE-CZ-NH1	-7.69	116.46	120.30
1	C	52	LEU	CA-CB-CG	7.64	132.87	115.30
1	K	166	ARG	NE-CZ-NH1	7.61	124.11	120.30
2	L	440	ARG	CB-CG-CD	-7.60	91.85	111.60
2	L	310	ILE	CG1-CB-CG2	-7.55	94.79	111.40
1	K	47	GLU	OE1-CD-OE2	7.52	132.32	123.30
1	A	147	ASP	CB-CG-OD1	7.52	125.07	118.30
2	B	362	ASP	CB-CG-OD2	7.51	125.06	118.30
1	I	106	LEU	CB-CG-CD2	-7.47	98.30	111.00
1	G	199	ASP	CB-CG-OD2	7.47	125.02	118.30
2	L	323	ASP	CB-CG-OD2	-7.43	111.61	118.30
2	D	457	ARG	NE-CZ-NH2	-7.42	116.59	120.30
1	I	5	LEU	CB-CG-CD2	-7.40	98.42	111.00
2	J	409	ARG	NE-CZ-NH2	-7.40	116.60	120.30
1	E	62	LEU	CB-CG-CD1	-7.39	98.44	111.00
1	A	174	ARG	NE-CZ-NH1	7.38	123.99	120.30
2	L	510	MET	CA-CB-CG	7.36	125.82	113.30
2	L	386	ASP	CB-CG-OD1	-7.35	111.69	118.30
2	J	483	ASP	CB-CG-OD1	-7.32	111.71	118.30
2	D	336	LEU	CB-CG-CD2	-7.30	98.59	111.00
2	L	330	ARG	NE-CZ-NH2	-7.29	116.66	120.30
2	L	447	TYR	CD1-CE1-CZ	-7.29	113.24	119.80
1	A	94	ARG	CD-NE-CZ	7.27	133.77	123.60
2	B	312	ASP	CB-CG-OD2	-7.21	111.81	118.30
2	D	527	LEU	CB-CG-CD1	-7.21	98.74	111.00
2	F	396	LEU	CB-CG-CD1	-7.21	98.74	111.00
1	G	55	VAL	CG1-CB-CG2	-7.17	99.42	110.90
2	J	447	TYR	CD1-CE1-CZ	-7.17	113.35	119.80
1	C	100	ASP	CB-CG-OD1	7.17	124.75	118.30
1	G	171	ILE	CG1-CB-CG2	-7.15	95.67	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	473	LYS	CD-CE-NZ	-7.15	95.26	111.70
2	F	531	ARG	NE-CZ-NH1	7.13	123.87	120.30
2	B	434	ASP	CB-CG-OD1	-7.13	111.89	118.30
1	C	142	ARG	NE-CZ-NH2	-7.12	116.74	120.30
1	E	189	ILE	CG1-CB-CG2	-7.09	95.79	111.40
2	B	413	ASP	CB-CG-OD1	7.08	124.67	118.30
1	E	167	ARG	NE-CZ-NH1	-7.05	116.78	120.30
2	L	430	LEU	CB-CG-CD2	-7.04	99.03	111.00
2	F	363	LEU	CB-CG-CD1	-7.03	99.06	111.00
1	G	146	ASP	CB-CG-OD2	7.03	124.62	118.30
2	D	362	ASP	CB-CG-OD1	-7.02	111.98	118.30
1	A	32	ASP	CB-CG-OD1	7.02	124.62	118.30
2	B	447	TYR	CD1-CE1-CZ	-7.00	113.50	119.80
2	J	447	TYR	OH-CZ-CE2	-7.00	101.21	120.10
1	C	184	ARG	NE-CZ-NH1	6.99	123.79	120.30
2	J	420	ASP	CB-CG-OD2	-6.97	112.03	118.30
2	B	420	ASP	CB-CG-OD1	6.96	124.56	118.30
1	I	114	VAL	CG1-CB-CG2	-6.94	99.79	110.90
1	E	168	GLU	OE1-CD-OE2	6.94	131.62	123.30
1	C	122	MET	CG-SD-CE	6.92	111.27	100.20
2	F	457	ARG	NH1-CZ-NH2	6.92	127.01	119.40
2	D	507	LYS	CD-CE-NZ	6.91	127.59	111.70
2	F	455	ASP	CB-CG-OD1	6.91	124.52	118.30
2	J	383	ARG	NE-CZ-NH1	6.91	123.75	120.30
1	K	180	LYS	N-CA-C	-6.91	92.36	111.00
1	K	187	ILE	CG1-CB-CG2	-6.87	96.29	111.40
1	A	184	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	G	106	LEU	CA-CB-CG	6.86	131.07	115.30
1	G	37	ASN	N-CA-C	6.83	129.43	111.00
2	H	428	ARG	CD-NE-CZ	6.81	133.14	123.60
1	C	183	TYR	CZ-CE2-CD2	-6.80	113.68	119.80
1	C	38	ARG	NE-CZ-NH2	-6.79	116.91	120.30
2	J	377	ARG	NE-CZ-NH2	6.78	123.69	120.30
1	E	65	ASP	CB-CG-OD2	-6.75	112.22	118.30
1	A	133	ARG	NE-CZ-NH2	-6.74	116.93	120.30
1	E	188	ARG	NH1-CZ-NH2	-6.73	112.00	119.40
2	B	521	TYR	CZ-CE2-CD2	-6.71	113.76	119.80
1	C	99	PHE	C-N-CA	6.70	138.44	121.70
2	L	307	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	G	4	LEU	CA-CB-CG	6.66	130.61	115.30
2	B	450	ARG	NE-CZ-NH1	-6.63	116.99	120.30
1	E	178	ASP	CB-CG-OD2	-6.63	112.34	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	94	ARG	CB-CG-CD	6.62	128.80	111.60
2	D	380	VAL	CG1-CB-CG2	-6.61	100.32	110.90
1	E	199	ASP	CB-CG-OD2	6.60	124.24	118.30
2	L	504	LEU	CB-CG-CD1	-6.58	99.81	111.00
1	G	122	MET	CG-SD-CE	6.58	110.72	100.20
2	D	323	ASP	CB-CG-OD1	6.57	124.21	118.30
2	D	414	ARG	NE-CZ-NH1	6.56	123.58	120.30
2	L	311	ARG	NE-CZ-NH1	-6.56	117.02	120.30
2	F	473	LYS	CD-CE-NZ	-6.55	96.63	111.70
1	E	3	GLU	CB-CA-C	-6.54	97.32	110.40
2	F	455	ASP	CB-CG-OD2	-6.53	112.42	118.30
2	D	340	PRO	CB-CA-C	-6.53	95.68	112.00
1	I	133	ARG	NE-CZ-NH2	-6.52	117.04	120.30
1	K	43	ASP	CB-CG-OD1	-6.52	112.43	118.30
2	B	384	VAL	CG1-CB-CG2	6.51	121.31	110.90
1	G	57	ASP	CB-CG-OD2	6.51	124.16	118.30
2	B	322	PRO	N-CA-C	6.50	129.01	112.10
2	B	478	LEU	CB-CG-CD1	-6.49	99.96	111.00
1	G	94	ARG	CD-NE-CZ	6.47	132.66	123.60
2	L	478	LEU	CA-CB-CG	6.43	130.10	115.30
2	D	531	ARG	NE-CZ-NH1	6.43	123.52	120.30
2	J	364	LEU	CB-CG-CD2	-6.43	100.07	111.00
2	J	508	LEU	CB-CG-CD1	-6.43	100.07	111.00
2	D	528	ARG	NE-CZ-NH2	-6.42	117.09	120.30
2	H	452	GLY	N-CA-C	-6.42	97.05	113.10
1	I	37	ASN	N-CA-C	6.41	128.31	111.00
2	F	517	ASP	CB-CG-OD1	6.41	124.07	118.30
1	K	32	ASP	CB-CG-OD1	-6.41	112.53	118.30
2	L	388	TYR	CE1-CZ-OH	-6.39	102.83	120.10
1	C	38	ARG	N-CA-CB	-6.39	99.10	110.60
2	D	407	ARG	NE-CZ-NH2	-6.37	117.11	120.30
2	B	455	ASP	CB-CG-OD2	-6.37	112.57	118.30
2	D	321	THR	N-CA-C	-6.35	93.85	111.00
2	J	311	ARG	NE-CZ-NH1	6.35	123.48	120.30
2	D	443	LYS	CD-CE-NZ	-6.34	97.11	111.70
2	L	362	ASP	CB-CG-OD1	6.34	124.00	118.30
1	G	38	ARG	CG-CD-NE	-6.34	98.49	111.80
1	I	38	ARG	NE-CZ-NH2	-6.34	117.13	120.30
2	L	325	LYS	CD-CE-NZ	-6.34	97.13	111.70
2	L	323	ASP	CB-CG-OD1	6.32	123.99	118.30
1	K	83	TYR	CB-CG-CD1	-6.31	117.21	121.00
1	C	196	VAL	CG1-CB-CG2	-6.28	100.86	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	524	ASP	CB-CG-OD2	-6.27	112.66	118.30
1	E	180	LYS	CD-CE-NZ	6.27	126.11	111.70
1	A	23	LEU	CA-CB-CG	6.26	129.71	115.30
2	H	372	LEU	CB-CG-CD1	6.26	121.64	111.00
2	F	451	ASN	CB-CA-C	6.25	122.91	110.40
2	H	407	ARG	NE-CZ-NH2	-6.24	117.18	120.30
2	B	493	LYS	CD-CE-NZ	6.24	126.04	111.70
1	C	69	GLU	OE1-CD-OE2	-6.22	115.84	123.30
1	C	114	VAL	CG1-CB-CG2	-6.22	100.95	110.90
1	G	43	ASP	CB-CG-OD2	-6.21	112.71	118.30
2	H	521	TYR	CD1-CE1-CZ	-6.21	114.21	119.80
1	K	21	LEU	CB-CG-CD2	-6.21	100.45	111.00
1	G	114	VAL	CG1-CB-CG2	-6.19	100.99	110.90
1	I	4	LEU	CB-CG-CD1	6.18	121.50	111.00
2	J	326	THR	OG1-CB-CG2	-6.18	95.79	110.00
1	C	154	LYS	CD-CE-NZ	6.17	125.90	111.70
2	H	321	THR	N-CA-C	-6.16	94.36	111.00
1	C	24	GLU	CA-CB-CG	6.16	126.95	113.40
2	B	416	LEU	CA-CB-CG	6.15	129.45	115.30
2	H	527	LEU	CB-CG-CD1	-6.15	100.54	111.00
1	G	187	ILE	CG1-CB-CG2	-6.14	97.90	111.40
1	G	68	LEU	CB-CG-CD1	-6.12	100.59	111.00
2	D	408[A]	CYS	CA-CB-SG	-6.12	102.99	114.00
2	D	408[B]	CYS	CA-CB-SG	-6.12	102.99	114.00
1	G	35	ILE	CG1-CB-CG2	-6.12	97.94	111.40
1	C	94	ARG	CB-CG-CD	6.10	127.47	111.60
2	H	528	ARG	NE-CZ-NH1	-6.10	117.25	120.30
1	I	162	GLU	OE1-CD-OE2	6.10	130.62	123.30
1	G	91	SER	N-CA-CB	-6.09	101.36	110.50
1	I	65	ASP	CB-CG-OD2	6.08	123.78	118.30
2	L	456	TRP	C-N-CA	-6.08	106.51	121.70
2	D	493	LYS	CD-CE-NZ	6.08	125.67	111.70
2	F	385	VAL	CG1-CB-CG2	-6.08	101.18	110.90
1	I	178	ASP	CB-CG-OD1	6.08	123.77	118.30
1	G	41	LYS	CD-CE-NZ	-6.07	97.73	111.70
2	L	388	TYR	OH-CZ-CE2	6.07	136.48	120.10
2	D	426	VAL	CB-CA-C	-6.06	99.88	111.40
2	B	312	ASP	CB-CG-OD1	6.06	123.75	118.30
2	L	527	LEU	CB-CG-CD1	-6.05	100.71	111.00
1	K	142	ARG	NE-CZ-NH2	-6.05	117.28	120.30
1	A	68	LEU	CA-CB-CG	6.04	129.20	115.30
1	I	94	ARG	CD-NE-CZ	6.04	132.06	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	146	ASP	N-CA-CB	6.04	121.47	110.60
2	J	307	ARG	NE-CZ-NH2	6.04	123.32	120.30
2	D	304	ASP	CB-CG-OD1	6.04	123.73	118.30
1	I	167	ARG	NE-CZ-NH1	6.03	123.32	120.30
2	D	425	GLY	CA-C-O	-6.03	109.75	120.60
2	B	524	ASP	CB-CG-OD1	6.02	123.72	118.30
2	J	312	ASP	CB-CG-OD2	-6.02	112.88	118.30
2	B	499	GLU	OE1-CD-OE2	6.02	130.52	123.30
2	F	443	LYS	CD-CE-NZ	6.02	125.54	111.70
1	K	64	ARG	NE-CZ-NH1	6.01	123.30	120.30
1	E	184	ARG	NE-CZ-NH1	6.00	123.30	120.30
2	D	386	ASP	CB-CG-OD2	5.99	123.69	118.30
1	K	103	GLU	CA-CB-CG	5.99	126.58	113.40
2	J	414	ARG	NE-CZ-NH2	-5.97	117.31	120.30
2	F	322	PRO	N-CA-C	5.97	127.62	112.10
2	J	360	ASP	CB-CG-OD1	5.96	123.67	118.30
2	J	307	ARG	NE-CZ-NH1	-5.95	117.32	120.30
2	F	416	LEU	CB-CG-CD1	5.95	121.11	111.00
2	J	450	ARG	NE-CZ-NH1	-5.95	117.33	120.30
1	C	166	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	E	43	ASP	CB-CG-OD1	-5.93	112.96	118.30
1	K	51	LEU	CB-CG-CD2	-5.93	100.92	111.00
1	K	143	LEU	CA-CB-CG	5.92	128.92	115.30
2	D	365	LEU	CB-CG-CD1	-5.92	100.94	111.00
2	F	416	LEU	CB-CG-CD2	-5.90	100.97	111.00
2	H	414	ARG	CA-CB-CG	5.90	126.38	113.40
2	D	362	ASP	CB-CG-OD2	5.89	123.61	118.30
2	L	516	MET	N-CA-CB	5.89	121.21	110.60
2	D	526	VAL	CG1-CB-CG2	5.89	120.33	110.90
2	D	415	TYR	CD1-CE1-CZ	-5.87	114.52	119.80
1	I	130	LEU	CB-CG-CD1	5.86	120.96	111.00
2	J	440	ARG	CB-CG-CD	-5.86	96.38	111.60
1	I	100	ASP	C-N-CA	5.85	136.33	121.70
1	K	38	ARG	CA-CB-CG	5.85	126.28	113.40
1	C	81	ASP	CB-CG-OD1	5.84	123.56	118.30
2	H	333	ARG	NE-CZ-NH2	-5.84	117.38	120.30
2	B	395	THR	CA-CB-CG2	5.84	120.58	112.40
1	C	21	LEU	CB-CG-CD1	5.83	120.91	111.00
2	F	437	TYR	CD1-CE1-CZ	-5.82	114.56	119.80
2	F	426	VAL	CG1-CB-CG2	-5.79	101.63	110.90
1	K	133	ARG	N-CA-CB	-5.79	100.18	110.60
2	F	538	CYS	CA-CB-SG	-5.78	103.59	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	133	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	E	64	ARG	NE-CZ-NH1	5.78	123.19	120.30
2	F	399	MET	CA-CB-CG	5.77	123.11	113.30
2	H	366	ASN	N-CA-C	5.77	126.58	111.00
2	J	447	TYR	CE1-CZ-OH	5.75	135.61	120.10
2	D	481	GLU	CG-CD-OE2	5.74	129.78	118.30
2	J	517	ASP	CB-CG-OD1	-5.74	113.13	118.30
1	A	41	LYS	CD-CE-NZ	-5.74	98.50	111.70
1	G	64	ARG	NE-CZ-NH2	-5.74	117.43	120.30
2	D	376	GLU	OE1-CD-OE2	5.71	130.16	123.30
2	F	383	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	A	94	ARG	CA-CB-CG	5.69	125.91	113.40
2	J	524	ASP	CB-CG-OD2	-5.67	113.19	118.30
2	H	416	LEU	CA-CB-CG	5.67	128.35	115.30
1	A	114	VAL	CG1-CB-CG2	-5.66	101.84	110.90
2	H	386	ASP	CB-CG-OD1	5.66	123.40	118.30
2	J	432	ASP	CB-CG-OD2	-5.66	113.20	118.30
2	J	434	ASP	CB-CG-OD1	-5.66	113.21	118.30
2	L	330	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	G	52	LEU	CA-CB-CG	5.65	128.29	115.30
1	I	143	LEU	CA-CB-CG	5.63	128.25	115.30
2	J	304	ASP	CB-CG-OD2	-5.63	113.23	118.30
2	B	383	ARG	NE-CZ-NH2	-5.63	117.48	120.30
2	D	474	LEU	CB-CG-CD2	-5.63	101.43	111.00
1	E	37	ASN	N-CA-C	5.63	126.19	111.00
1	G	142	ARG	CB-CG-CD	-5.62	96.99	111.60
2	H	427	GLY	CA-C-O	-5.61	110.50	120.60
2	J	538	CYS	CA-CB-SG	-5.61	103.89	114.00
1	C	183	TYR	CB-CG-CD1	-5.61	117.63	121.00
2	L	451	ASN	N-CA-C	-5.60	95.88	111.00
1	I	147	ASP	CB-CG-OD1	5.59	123.34	118.30
2	D	320	LEU	CB-CG-CD1	5.58	120.49	111.00
2	F	323	ASP	CB-CG-OD1	5.58	123.32	118.30
2	B	453	PRO	N-CD-CG	-5.57	94.84	103.20
2	H	457	ARG	CB-CG-CD	5.57	126.09	111.60
2	J	320	LEU	CB-CG-CD1	5.57	120.47	111.00
2	J	348	GLY	N-CA-C	-5.56	99.19	113.10
1	C	192	GLU	N-CA-CB	-5.55	100.61	110.60
2	J	495	ILE	CG1-CB-CG2	5.55	123.61	111.40
1	K	186	ASP	CB-CG-OD1	5.54	123.29	118.30
2	F	528	ARG	NH1-CZ-NH2	5.53	125.48	119.40
2	H	507	LYS	CD-CE-NZ	5.52	124.40	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	63	VAL	CG1-CB-CG2	-5.52	102.07	110.90
2	H	324	TYR	CB-CG-CD1	5.51	124.30	121.00
2	B	495	ILE	CB-CA-C	-5.50	100.60	111.60
2	H	379	ILE	CB-CA-C	-5.50	100.60	111.60
2	F	430	LEU	CB-CG-CD2	-5.50	101.65	111.00
1	E	94	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	I	68	LEU	CA-CB-CG	5.49	127.94	115.30
2	D	457	ARG	CG-CD-NE	5.48	123.31	111.80
1	I	4	LEU	CB-CG-CD2	-5.47	101.70	111.00
2	J	467	GLY	C-N-CD	5.47	139.88	128.40
2	D	310	ILE	CG1-CB-CG2	-5.46	99.38	111.40
1	G	68	LEU	CA-CB-CG	5.46	127.87	115.30
2	D	538	CYS	N-CA-C	5.46	125.75	111.00
1	G	147	ASP	CB-CG-OD1	5.46	123.21	118.30
1	K	74	ASP	CB-CG-OD2	-5.45	113.39	118.30
2	F	377	ARG	NE-CZ-NH2	5.44	123.02	120.30
1	I	94	ARG	CA-CB-CG	5.43	125.36	113.40
1	K	78	GLU	OE1-CD-OE2	5.42	129.81	123.30
2	B	457	ARG	CG-CD-NE	5.41	123.16	111.80
1	C	135	ILE	CG1-CB-CG2	5.41	123.30	111.40
1	A	200	PHE	CZ-CE2-CD2	5.41	126.59	120.10
2	B	364	LEU	CB-CG-CD1	5.40	120.18	111.00
2	H	325	LYS	CD-CE-NZ	-5.40	99.28	111.70
1	C	94	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	G	31	ARG	NE-CZ-NH2	5.39	123.00	120.30
2	L	376	GLU	OE1-CD-OE2	5.39	129.77	123.30
2	H	324	TYR	CB-CG-CD2	-5.39	117.77	121.00
1	A	23	LEU	CB-CG-CD2	-5.38	101.85	111.00
2	J	323	ASP	N-CA-CB	-5.37	100.94	110.60
1	C	180	LYS	CB-CA-C	5.36	121.11	110.40
1	E	38	ARG	NH1-CZ-NH2	-5.35	113.52	119.40
1	E	167	ARG	NE-CZ-NH2	5.34	122.97	120.30
1	A	38	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	I	178	ASP	CB-CG-OD2	-5.32	113.51	118.30
2	H	498	PRO	CB-CG-CD	-5.32	85.75	106.50
2	H	463	PHE	CB-CA-C	-5.32	99.77	110.40
1	C	91	SER	N-CA-CB	-5.31	102.53	110.50
2	D	379	ILE	CG1-CB-CG2	-5.31	99.72	111.40
2	F	385	VAL	CA-CB-CG1	-5.31	102.94	110.90
2	L	479	TYR	CA-CB-CG	-5.30	103.33	113.40
1	C	32	ASP	CB-CG-OD2	5.30	123.07	118.30
2	D	451	ASN	N-CA-C	-5.30	96.69	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	103	GLU	OE1-CD-OE2	5.29	129.65	123.30
2	L	371	GLY	N-CA-C	5.29	126.33	113.10
2	H	384	VAL	CG1-CB-CG2	-5.28	102.44	110.90
2	B	378	ILE	CG1-CB-CG2	-5.28	99.78	111.40
1	G	199	ASP	CB-CG-OD1	-5.28	113.55	118.30
1	E	160	LEU	CB-CG-CD1	-5.27	102.04	111.00
2	L	388	TYR	CB-CG-CD2	5.27	124.16	121.00
1	K	36	TRP	CB-CA-C	5.26	120.93	110.40
1	K	106	LEU	CA-CB-CG	5.26	127.40	115.30
1	C	38	ARG	CG-CD-NE	-5.26	100.76	111.80
1	I	184	ARG	NE-CZ-NH1	5.25	122.93	120.30
1	I	188	ARG	NE-CZ-NH2	-5.25	117.68	120.30
2	H	428	ARG	CB-CA-C	-5.24	99.91	110.40
2	B	337	VAL	CA-CB-CG2	-5.24	103.04	110.90
2	H	505	ILE	CA-CB-CG1	5.24	120.95	111.00
2	H	411	LYS	CB-CA-C	-5.24	99.93	110.40
2	H	390	LYS	CD-CE-NZ	-5.23	99.67	111.70
2	F	317	PRO	O-C-N	-5.22	114.34	122.70
2	H	427	GLY	CA-C-N	5.22	128.68	117.20
1	G	106	LEU	CB-CG-CD1	5.21	119.86	111.00
2	J	464	GLY	N-CA-C	-5.21	100.06	113.10
1	I	143	LEU	CB-CG-CD2	-5.21	102.14	111.00
1	K	116	ASN	CB-CA-C	5.21	120.83	110.40
2	B	483	ASP	CB-CG-OD1	5.21	122.99	118.30
2	L	507	LYS	CD-CE-NZ	5.21	123.67	111.70
2	H	470	ILE	CB-CG1-CD1	-5.20	99.34	113.90
1	E	10	SER	N-CA-CB	-5.20	102.70	110.50
2	D	447	TYR	CD1-CE1-CZ	-5.20	115.12	119.80
2	L	517	ASP	N-CA-CB	-5.19	101.25	110.60
1	C	140	HIS	CB-CA-C	-5.19	100.02	110.40
2	H	426	VAL	CA-CB-CG2	-5.19	103.11	110.90
2	H	504	LEU	CB-CG-CD1	-5.19	102.18	111.00
1	C	74	ASP	CB-CG-OD1	5.19	122.97	118.30
2	D	306	SER	CA-CB-OG	-5.19	97.19	111.20
1	G	9	PRO	CB-CA-C	-5.18	99.05	112.00
2	B	380	VAL	N-CA-C	-5.18	97.02	111.00
1	K	64	ARG	NE-CZ-NH2	-5.17	117.71	120.30
2	L	517	ASP	CB-CG-OD1	5.17	122.96	118.30
1	G	178	ASP	CB-CG-OD2	5.17	122.95	118.30
1	C	69	GLU	CG-CD-OE2	5.17	128.63	118.30
2	F	321	THR	N-CA-C	-5.17	97.05	111.00
2	B	447	TYR	OH-CZ-CE2	-5.16	106.18	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	333	ARG	NE-CZ-NH1	-5.15	117.72	120.30
1	C	101	ALA	CA-C-N	5.15	126.49	116.20
1	E	157	VAL	CG1-CB-CG2	5.15	119.14	110.90
1	I	52	LEU	CA-CB-CG	5.15	127.14	115.30
2	F	414	ARG	NE-CZ-NH2	-5.14	117.73	120.30
2	J	366	ASN	N-CA-C	5.14	124.88	111.00
2	H	440	ARG	CD-NE-CZ	5.14	130.79	123.60
2	F	324	TYR	N-CA-C	-5.13	97.14	111.00
2	B	379	ILE	CG1-CB-CG2	-5.12	100.12	111.40
2	J	420	ASP	CB-CG-OD1	5.12	122.91	118.30
2	D	306	SER	N-CA-CB	-5.11	102.84	110.50
1	K	167	ARG	NE-CZ-NH1	-5.11	117.75	120.30
2	B	372	LEU	CB-CG-CD1	5.10	119.67	111.00
2	H	304	ASP	CB-CG-OD2	-5.10	113.71	118.30
2	D	379	ILE	CA-CB-CG1	5.10	120.68	111.00
2	H	447	TYR	CB-CG-CD2	-5.10	117.94	121.00
1	A	50	LEU	CB-CG-CD1	-5.09	102.35	111.00
1	A	89	PHE	CB-CG-CD1	-5.09	117.24	120.80
2	L	419	LEU	CB-CG-CD2	-5.09	102.35	111.00
2	B	347	THR	CA-CB-CG2	-5.08	105.29	112.40
2	D	479	TYR	CD1-CE1-CZ	5.08	124.37	119.80
2	J	365	LEU	CB-CG-CD1	-5.08	102.37	111.00
2	F	416	LEU	CA-CB-CG	5.07	126.95	115.30
2	B	379	ILE	N-CA-C	-5.06	97.33	111.00
2	B	397	VAL	CG1-CB-CG2	-5.06	102.80	110.90
2	J	519	LEU	CA-CB-CG	-5.06	103.65	115.30
1	E	158	LEU	CB-CG-CD1	5.06	119.60	111.00
1	G	16	TYR	CB-CG-CD1	-5.06	117.96	121.00
2	D	335	ALA	N-CA-CB	-5.06	103.02	110.10
2	H	435	GLY	CA-C-O	-5.06	111.50	120.60
2	J	517	ASP	N-CA-CB	-5.06	101.50	110.60
2	D	337	VAL	CA-CB-CG2	-5.05	103.32	110.90
2	H	508	LEU	CB-CG-CD1	-5.04	102.43	111.00
2	B	451	ASN	N-CA-C	-5.04	97.39	111.00
2	D	368	ASN	CA-C-N	-5.04	106.11	117.20
2	D	450	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	K	66	SER	CA-CB-OG	-5.04	97.60	111.20
2	L	350	ASN	N-CA-C	-5.04	97.41	111.00
2	L	472	THR	CB-CA-C	-5.03	98.01	111.60
2	B	473	LYS	CB-CA-C	5.03	120.47	110.40
2	H	390	LYS	N-CA-CB	-5.03	101.56	110.60
2	H	465	ILE	CG1-CB-CG2	5.02	122.45	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	522	ARG	CG-CD-NE	-5.02	101.26	111.80
1	K	43	ASP	CB-CG-OD2	5.02	122.82	118.30
2	H	324	TYR	N-CA-C	-5.01	97.47	111.00

There are no chirality outliers.

All (116) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	134	GLY	Mainchain
1	A	144	TYR	Sidechain
1	A	16	TYR	Sidechain
1	A	166	ARG	Sidechain
1	A	192	GLU	Mainchain
1	A	44	ALA	Mainchain
1	A	83	TYR	Sidechain
2	B	354	LEU	Mainchain
2	B	383	ARG	Sidechain
2	B	395	THR	Mainchain
2	B	408[A]	CYS	Mainchain
2	B	409	ARG	Mainchain
2	B	437	TYR	Sidechain
2	B	440	ARG	Sidechain
2	B	465	ILE	Mainchain
2	B	527	LEU	Mainchain
2	B	531	ARG	Sidechain
1	C	138	HIS	Mainchain
1	C	139	LEU	Mainchain
1	C	156	PRO	Mainchain
1	C	16	TYR	Sidechain
1	C	18	HIS	Sidechain
1	C	180	LYS	Mainchain
1	C	184	ARG	Mainchain
1	C	56	TYR	Sidechain
1	C	69	GLU	Mainchain
1	C	99	PHE	Mainchain
2	D	311	ARG	Sidechain,Mainchain
2	D	324	TYR	Mainchain
2	D	325	LYS	Mainchain
2	D	334	GLN	Mainchain
2	D	351	PHE	Mainchain
2	D	391	PRO	Mainchain
2	D	407	ARG	Sidechain

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Mol	Chain	Res	Type	Group
2	D	410	HIS	Mainchain
2	D	467	GLY	Mainchain
2	D	471	ALA	Mainchain
2	D	493	LYS	Mainchain
2	D	511	ASN	Sidechain
2	D	525	ILE	Mainchain
2	D	528	ARG	Sidechain
1	E	16	TYR	Sidechain
1	E	166	ARG	Sidechain
1	E	64	ARG	Mainchain
1	E	99	PHE	Mainchain
2	F	353	HIS	Sidechain
2	F	366	ASN	Mainchain
2	F	430	LEU	Mainchain
2	F	440	ARG	Sidechain
2	F	447	TYR	Sidechain
2	F	465	ILE	Mainchain
1	G	1	PRO	Mainchain
1	G	18	HIS	Mainchain
1	G	184	ARG	Mainchain
1	G	187	ILE	Mainchain
1	G	37	ASN	Mainchain
1	G	38	ARG	Sidechain
1	G	96	ALA	Mainchain
2	H	313	ARG	Mainchain
2	H	336	LEU	Mainchain
2	H	341	GLN	Mainchain
2	H	354	LEU	Mainchain
2	H	360	ASP	Mainchain
2	H	407	ARG	Sidechain
2	H	428	ARG	Mainchain
2	H	436	TYR	Sidechain
2	H	447	TYR	Sidechain
2	H	525	ILE	Mainchain
1	I	11	GLN	Mainchain
1	I	133	ARG	Sidechain
1	I	18	HIS	Mainchain
1	I	184	ARG	Sidechain
1	I	53	GLY	Mainchain
1	I	69	GLU	Mainchain
1	I	95	THR	Mainchain
2	J	313	ARG	Sidechain

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Mol	Chain	Res	Type	Group
2	J	317	PRO	Mainchain
2	J	341	GLN	Mainchain
2	J	344	SER	Mainchain
2	J	384	VAL	Mainchain
2	J	391	PRO	Mainchain
2	J	407	ARG	Sidechain
2	J	415	TYR	Sidechain
2	J	447	TYR	Sidechain
2	J	451	ASN	Mainchain
2	J	466	SER	Mainchain
2	J	505	ILE	Mainchain
2	J	511	ASN	Sidechain
2	J	516	MET	Mainchain
2	J	520	ALA	Mainchain
2	J	529	GLY	Mainchain
1	K	144	TYR	Sidechain
1	K	183	TYR	Sidechain
1	K	56	TYR	Sidechain
1	K	74	ASP	Mainchain
1	K	83	TYR	Sidechain
1	K	90	ASN	Mainchain
2	L	309	VAL	Mainchain
2	L	342	SER	Mainchain
2	L	353	HIS	Sidechain
2	L	360	ASP	Mainchain
2	L	362	ASP	Mainchain
2	L	388	TYR	Sidechain
2	L	390	LYS	Mainchain
2	L	423	PHE	Mainchain
2	L	447	TYR	Sidechain
2	L	468	PRO	Mainchain
2	L	479	TYR	Sidechain
2	L	484	PRO	Mainchain
2	L	487	PRO	Mainchain
2	L	506	ALA	Mainchain
2	L	509	ASP	Mainchain
2	L	516	MET	Mainchain
2	L	521	TYR	Sidechain
2	L	533	THR	Mainchain

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	20	0
1	C	1571	0	1499	27	0
1	E	1571	0	1499	33	0
1	G	1571	0	1499	21	0
1	I	1571	0	1499	32	0
1	K	1571	0	1499	38	0
2	B	1875	0	1821	49	1
2	D	1875	0	1821	48	0
2	F	1875	0	1821	42	1
2	H	1875	0	1821	37	1
2	J	1875	0	1821	47	0
2	L	1875	0	1821	43	1
3	B	1	0	0	0	0
3	D	1	0	0	0	0
3	F	1	0	0	0	0
3	H	1	0	0	0	0
3	J	1	0	0	0	0
3	L	1	0	0	0	0
4	B	11	0	4	3	0
4	D	11	0	5	2	0
4	F	11	0	3	5	0
4	H	11	0	4	3	0
4	J	11	0	4	3	0
4	L	11	0	5	4	0
5	A	51	0	0	1	0
5	B	111	0	0	5	0
5	C	49	0	0	1	0
5	D	122	0	0	2	1
5	E	54	0	0	0	0
5	F	113	0	0	3	1
5	G	52	0	0	0	0
5	H	108	0	0	5	0
5	I	55	0	0	1	0
5	J	115	0	0	5	1
5	K	48	0	0	1	0
5	L	118	0	0	3	1
All	All	21744	0	19945	395	4

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 10.

All (395) 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)
2:L:337:VAL:CG1	2:L:337:VAL:CB	1.74	1.62
2:B:339:ILE:CD1	2:B:339:ILE:CG1	1.74	1.60
1:G:154:LYS:CE	1:G:154:LYS:CD	1.76	1.60
2:F:390:LYS:CG	2:F:390:LYS:CD	1.78	1.59
2:H:396:LEU:CG	2:H:396:LEU:CD1	1.79	1.59
2:J:378:ILE:CG1	2:J:378:ILE:CD1	1.76	1.58
1:E:157:VAL:CB	1:E:157:VAL:CG1	1.75	1.57
2:L:303:GLN:CB	2:L:303:GLN:CA	1.75	1.56
2:B:453:PRO:CG	2:B:453:PRO:CB	1.77	1.56
1:A:154:LYS:CD	1:A:154:LYS:CE	1.74	1.56
1:I:154:LYS:CE	1:I:154:LYS:NZ	1.68	1.55
2:J:493:LYS:CE	2:J:493:LYS:NZ	1.70	1.54
2:D:493:LYS:NZ	2:D:493:LYS:CE	1.68	1.52
2:B:303:GLN:CA	2:B:303:GLN:CB	1.86	1.51
1:C:154:LYS:NZ	1:C:154:LYS:CE	1.70	1.51
2:D:515:PRO:CB	2:D:515:PRO:CG	1.76	1.50
2:L:507:LYS:CE	2:L:507:LYS:NZ	1.76	1.49
1:A:154:LYS:NZ	1:A:154:LYS:CE	1.74	1.48
1:G:9:PRO:CG	1:G:9:PRO:CD	1.75	1.47
2:D:408[B]:CYS:SG	2:D:408[B]:CYS:CB	2.04	1.45
2:H:498:PRO:CG	2:H:498:PRO:CB	1.79	1.45
2:J:448:PRO:CG	2:J:448:PRO:CB	1.80	1.45
2:F:507:LYS:NZ	2:F:507:LYS:CE	1.75	1.44
2:B:489:CYS:SG	2:B:489:CYS:CB	2.04	1.43
2:B:507:LYS:CE	2:B:507:LYS:NZ	1.76	1.43
2:J:317:PRO:CG	2:J:317:PRO:CB	1.75	1.42
1:K:42:PRO:CB	1:K:42:PRO:CG	1.78	1.41
2:D:507:LYS:CE	2:D:507:LYS:NZ	1.85	1.38
2:D:510:MET:SD	2:D:510:MET:CE	2.17	1.31
1:K:165:GLN:NE2	1:K:165:GLN:H	1.43	1.17
2:H:364:LEU:HD22	2:H:440:ARG:HD3	1.22	1.10
1:I:165:GLN:N	1:I:165:GLN:HE21	1.49	1.09
1:I:165:GLN:H	1:I:165:GLN:NE2	1.54	1.05
2:D:368:ASN:ND2	2:D:370:GLY:H	1.59	1.01
1:E:165:GLN:H	1:E:165:GLN:HE21	1.05	1.00
1:C:165:GLN:H	1:C:165:GLN:HE21	1.04	0.93
1:K:165:GLN:N	1:K:165:GLN:HE21	1.66	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:368:ASN:ND2	2:H:370:GLY:H	1.68	0.93
1:K:165:GLN:HE21	1:K:165:GLN:H	0.89	0.88
1:E:165:GLN:NE2	1:E:165:GLN:H	1.70	0.87
1:C:26:ALA:O	2:D:411:LYS:NZ	2.06	0.87
2:F:408[A]:CYS:SG	5:F:2901:HOH:O	2.35	0.85
2:B:497:ASN:HD22	2:B:497:ASN:C	1.80	0.84
1:E:25:ALA:HB1	1:E:98:THR:HG21	1.61	0.83
1:I:25:ALA:HB1	1:I:98:THR:HG21	1.61	0.81
1:C:165:GLN:H	1:C:165:GLN:NE2	1.78	0.81
2:D:368:ASN:ND2	2:D:370:GLY:N	2.30	0.79
2:J:538:CYS:OXT	5:J:833:HOH:O	1.99	0.79
2:B:390:LYS:HD3	5:B:677:HOH:O	1.83	0.78
2:J:408[A]:CYS:SG	5:J:4901:HOH:O	2.42	0.76
1:E:26:ALA:O	2:F:411:LYS:NZ	2.19	0.76
2:B:497:ASN:HD22	2:B:498:PRO:N	1.84	0.76
1:C:98:THR:N	1:C:101:ALA:O	2.19	0.75
1:E:157:VAL:CG1	1:E:157:VAL:CA	2.65	0.74
2:H:408[A]:CYS:SG	5:H:3901:HOH:O	2.44	0.74
2:F:361:HIS:CD2	2:F:361:HIS:H	2.05	0.73
2:D:447:TYR:OH	4:D:1550:DHB:O4	2.07	0.73
1:E:165:GLN:N	1:E:165:GLN:HE21	1.85	0.73
1:A:165:GLN:H	1:A:165:GLN:NE2	1.86	0.73
2:D:510:MET:CG	2:D:510:MET:CE	2.67	0.73
2:F:497:ASN:ND2	2:F:499:GLU:H	1.87	0.72
2:L:337:VAL:CG1	2:L:337:VAL:CG2	2.67	0.72
1:K:67:PHE:HZ	1:K:94:ARG:HD2	1.55	0.72
1:G:67:PHE:CZ	1:G:94:ARG:HD2	2.25	0.71
2:H:396:LEU:CB	2:H:396:LEU:CD1	2.69	0.71
2:F:324:TYR:OH	4:F:2550:DHB:O1	2.07	0.71
1:K:165:GLN:N	1:K:165:GLN:NE2	2.28	0.70
1:I:51:LEU:HD12	1:I:106:LEU:HD23	1.73	0.69
1:K:67:PHE:CZ	1:K:94:ARG:HD2	2.28	0.69
2:L:337:VAL:CA	2:L:337:VAL:CG1	2.69	0.68
1:K:110:LYS:NZ	1:K:148:GLU:OE2	2.20	0.68
2:D:361:HIS:H	2:D:361:HIS:CD2	2.11	0.68
2:L:361:HIS:H	2:L:361:HIS:CD2	2.12	0.67
1:C:165:GLN:N	1:C:165:GLN:HE21	1.86	0.67
2:L:368:ASN:O	2:L:369:ASN:ND2	2.27	0.67
2:L:411:LYS:CE	2:L:411:LYS:H	2.08	0.67
2:H:376:GLU:OE1	5:H:3665:HOH:O	2.13	0.67
2:L:447:TYR:HE1	4:L:5550:DHB:H5	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:468:PRO:HD2	2:L:472:THR:HG21	1.76	0.67
1:G:154:LYS:CE	1:G:154:LYS:CG	2.71	0.66
1:E:51:LEU:HD12	1:E:106:LEU:HD23	1.77	0.66
2:D:368:ASN:HD21	2:D:370:GLY:H	1.40	0.66
2:H:368:ASN:ND2	2:H:370:GLY:N	2.43	0.66
2:F:368:ASN:HD22	2:F:370:GLY:H	1.44	0.66
1:C:24:GLU:O	1:C:27:GLY:N	2.24	0.65
2:B:393:PRO:O	5:B:779:HOH:O	2.12	0.65
2:B:339:ILE:CD1	2:B:339:ILE:CB	2.70	0.65
2:D:368:ASN:HD21	2:D:370:GLY:CA	2.09	0.65
2:H:325:LYS:HD3	2:J:335:ALA:HB1	1.79	0.65
2:F:497:ASN:HD22	2:F:499:GLU:H	1.45	0.64
1:K:15:PRO:HB3	1:K:133:ARG:HD2	1.78	0.64
2:H:361:HIS:CD2	2:H:361:HIS:H	2.16	0.64
1:I:54:GLN:O	5:I:4754:HOH:O	2.15	0.63
1:I:24:GLU:O	1:I:27:GLY:N	2.31	0.63
1:A:154:LYS:CG	1:A:154:LYS:CE	2.75	0.63
1:G:67:PHE:HZ	1:G:94:ARG:HD2	1.63	0.63
2:L:447:TYR:OH	4:L:5550:DHB:O4	2.17	0.63
2:D:465:ILE:HG13	2:D:525:ILE:HG21	1.80	0.63
2:F:390:LYS:HD2	5:F:2677:HOH:O	1.99	0.62
2:B:408[A]:CYS:SG	5:B:901:HOH:O	2.42	0.62
2:D:416:LEU:H	2:D:416:LEU:HD23	1.64	0.62
1:I:161:ILE:HD13	1:I:196:VAL:HG21	1.82	0.62
2:H:368:ASN:HD22	2:H:370:GLY:H	1.48	0.62
1:K:143:LEU:C	1:K:143:LEU:HD23	2.19	0.61
2:B:361:HIS:CD2	2:B:361:HIS:H	2.16	0.61
2:J:453:PRO:HB2	2:L:310:ILE:HG12	1.81	0.61
2:D:482:GLY:O	5:D:1704:HOH:O	2.16	0.61
2:D:510:MET:HG3	2:D:510:MET:CE	2.30	0.61
2:D:447:TYR:HE1	4:D:1550:DHB:H5	1.65	0.60
1:G:165:GLN:HE21	1:G:165:GLN:H	1.49	0.60
1:K:64:ARG:NH1	5:K:5903:HOH:O	2.31	0.60
1:I:94:ARG:NH2	2:J:398:GLU:OE2	2.33	0.60
1:G:70:VAL:HG11	1:G:106:LEU:HD21	1.83	0.60
1:C:67:PHE:HZ	1:C:94:ARG:HD2	1.66	0.59
2:F:497:ASN:HD22	2:F:497:ASN:C	2.05	0.59
2:L:376:GLU:OE1	5:L:5665:HOH:O	2.16	0.59
2:J:390:LYS:HD2	5:J:4677:HOH:O	2.02	0.59
2:H:453:PRO:HB2	2:J:310:ILE:HG12	1.84	0.59
2:D:368:ASN:HD21	2:D:370:GLY:N	1.96	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:497:ASN:HD22	2:J:499:GLU:H	1.51	0.59
2:B:497:ASN:ND2	2:B:499:GLU:H	2.02	0.58
2:F:447:TYR:OH	4:F:2550:DHB:O4	2.21	0.58
1:E:157:VAL:HB	1:E:157:VAL:CG1	2.17	0.58
2:B:497:ASN:C	2:B:497:ASN:ND2	2.52	0.58
2:L:364:LEU:HD22	2:L:440:ARG:HD3	1.86	0.58
2:L:497:ASN:ND2	2:L:499:GLU:H	2.01	0.58
2:L:411:LYS:HE2	2:L:411:LYS:H	1.68	0.58
2:J:361:HIS:H	2:J:361:HIS:CD2	2.21	0.58
1:E:111:PRO:HD2	1:E:145:PHE:CZ	2.40	0.57
2:L:315:TRP:HZ2	2:L:503:GLN:HE21	1.53	0.57
2:H:411:LYS:NZ	2:H:411:LYS:H	2.03	0.56
2:L:497:ASN:HD22	2:L:498:PRO:N	2.04	0.56
1:K:17:VAL:CG2	1:K:21:LEU:HD12	2.35	0.56
2:H:429:CYS:SG	5:H:3766:HOH:O	2.19	0.56
2:H:396:LEU:CD1	2:H:396:LEU:CD2	2.74	0.56
1:A:26:ALA:O	2:B:411:LYS:NZ	2.36	0.55
2:H:411:LYS:O	2:H:414:ARG:NH1	2.40	0.55
1:E:80:GLN:O	1:E:91:SER:HB2	2.07	0.55
2:L:408[A]:CYS:SG	5:L:5901:HOH:O	2.45	0.55
2:J:447:TYR:HE1	4:J:4550:DHB:H5	1.71	0.55
2:J:368:ASN:ND2	2:J:370:GLY:H	2.05	0.55
2:J:495:ILE:HG21	2:J:500:ALA:HB3	1.87	0.55
2:J:364:LEU:HD22	2:J:440:ARG:HD3	1.89	0.55
2:B:367:PHE:O	2:B:368:ASN:O	2.24	0.54
1:G:165:GLN:NE2	1:G:165:GLN:H	2.06	0.54
2:B:364:LEU:HD22	2:B:440:ARG:HD3	1.88	0.54
2:F:368:ASN:ND2	2:F:370:GLY:H	2.05	0.54
2:H:497:ASN:HD22	2:H:499:GLU:H	1.55	0.54
2:B:310:ILE:HG13	2:F:453:PRO:HB2	1.90	0.54
2:H:345:GLU:HA	2:H:470:ILE:HD11	1.90	0.53
2:B:507:LYS:HB2	1:I:2:ILE:HD13	1.90	0.53
2:J:394:ASN:HB3	2:J:430:LEU:HD21	1.90	0.53
2:H:497:ASN:ND2	2:H:499:GLU:H	2.07	0.53
1:C:19:ILE:HG21	2:D:410:HIS:HB2	1.90	0.53
1:A:165:GLN:H	1:A:165:GLN:HE21	1.56	0.53
2:F:497:ASN:HD22	2:F:498:PRO:N	2.07	0.53
2:J:371:GLY:H	2:J:422:ASN:ND2	2.07	0.53
1:I:26:ALA:O	2:J:411:LYS:NZ	2.40	0.53
2:B:453:PRO:HB2	2:D:310:ILE:HG13	1.89	0.53
2:L:447:TYR:CZ	4:L:5550:DHB:O4	2.59	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:449:TRP:CD1	2:H:449:TRP:N	2.76	0.53
1:E:92:PHE:CD1	2:F:349:PRO:HG3	2.45	0.52
1:I:127:ASN:HD21	2:J:344:SER:HB3	1.74	0.52
2:F:356:PHE:CD1	2:F:428:ARG:HD3	2.43	0.52
1:A:70:VAL:HA	1:A:127:ASN:O	2.09	0.52
2:J:376:GLU:O	2:J:442:ILE:HA	2.09	0.52
1:E:157:VAL:C	1:E:157:VAL:CG1	2.78	0.52
2:B:315:TRP:HZ2	2:B:503:GLN:NE2	2.07	0.52
2:L:497:ASN:HD22	2:L:497:ASN:C	2.13	0.52
1:G:15:PRO:HD3	4:H:3550:DHB:C1	2.40	0.52
1:E:15:PRO:HB3	1:E:133:ARG:HD2	1.93	0.51
1:I:20:GLY:HA2	2:J:426:VAL:HG13	1.93	0.51
2:F:449:TRP:N	2:F:449:TRP:CD1	2.78	0.51
2:F:390:LYS:CB	2:F:390:LYS:CD	2.80	0.51
2:D:368:ASN:HD21	2:D:370:GLY:HA2	1.74	0.51
2:J:497:ASN:ND2	2:J:499:GLU:H	2.07	0.51
2:H:386:ASP:HB2	2:H:529:GLY:HA2	1.91	0.51
2:B:315:TRP:HZ2	2:B:503:GLN:HE21	1.58	0.51
2:J:447:TYR:CZ	4:J:4550:DHB:O4	2.64	0.51
2:B:364:LEU:HD22	2:B:440:ARG:CD	2.40	0.51
2:L:385:VAL:O	2:L:526:VAL:HA	2.11	0.51
1:K:174:ARG:HH21	1:K:181:THR:HG21	1.75	0.51
2:B:411:LYS:H	2:B:411:LYS:HZ3	1.59	0.50
1:A:39:LEU:HD11	1:A:93:GLY:HA3	1.93	0.50
2:B:448:PRO:HD3	2:B:456:TRP:CZ3	2.45	0.50
2:B:324:TYR:OH	4:B:550:DHB:O1	2.21	0.50
1:E:110:LYS:HE3	1:E:183:TYR:OH	2.11	0.50
1:I:165:GLN:H	1:I:165:GLN:HE21	0.71	0.50
2:B:368:ASN:HD22	2:B:370:GLY:H	1.59	0.50
2:H:497:ASN:C	2:H:497:ASN:HD22	2.15	0.50
1:C:19:ILE:CG2	2:D:410:HIS:HB2	2.41	0.50
1:I:67:PHE:HZ	1:I:94:ARG:HD2	1.77	0.50
1:C:131:PHE:CD2	2:D:475:ILE:HD12	2.46	0.50
1:K:18:HIS:HB2	1:K:26:ALA:HB2	1.93	0.50
1:G:65:ASP:OD2	1:G:133:ARG:HD3	2.11	0.50
1:K:30:THR:HG22	1:K:34:GLU:HG3	1.93	0.50
1:I:65:ASP:OD2	1:I:133:ARG:HD3	2.12	0.50
2:J:448:PRO:HD3	2:J:456:TRP:CZ3	2.47	0.50
1:A:114:VAL:HG22	5:A:680:HOH:O	2.12	0.50
1:G:131:PHE:O	1:G:132:ALA:HB2	2.12	0.50
1:I:131:PHE:CE2	1:I:138:HIS:HB3	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:39:LEU:HD11	1:I:93:GLY:HA3	1.94	0.50
1:A:18:HIS:HA	1:A:22:ALA:HB3	1.92	0.50
2:H:368:ASN:HD22	2:H:369:ASN:N	2.10	0.50
1:K:195:THR:HG22	1:K:196:VAL:O	2.12	0.50
2:B:400:TRP:HA	2:B:425:GLY:O	2.12	0.50
2:D:411:LYS:NZ	2:D:411:LYS:H	2.11	0.49
2:D:447:TYR:HB2	2:D:448:PRO:HD2	1.94	0.49
2:L:497:ASN:HD22	2:L:499:GLU:H	1.59	0.49
1:C:11:GLN:NE2	2:D:495:ILE:HD11	2.26	0.49
2:F:429:CYS:SG	5:F:2766:HOH:O	1.93	0.49
1:I:49:ILE:HD13	1:I:110:LYS:N	2.28	0.49
1:C:18:HIS:HA	1:C:22:ALA:HB3	1.93	0.49
2:B:320:LEU:HD22	2:B:333:ARG:CZ	2.42	0.49
2:F:478:LEU:C	2:F:478:LEU:HD23	2.33	0.49
1:C:170:LEU:HD21	1:C:196:VAL:HB	1.95	0.49
1:C:25:ALA:HB1	1:C:98:THR:HG21	1.93	0.49
1:K:98:THR:N	1:K:101:ALA:O	2.40	0.49
2:F:315:TRP:HZ2	2:F:503:GLN:NE2	2.11	0.49
2:D:368:ASN:ND2	2:D:371:GLY:H	2.10	0.49
2:H:368:ASN:HD21	2:H:370:GLY:H	1.56	0.49
1:K:92:PHE:CD1	2:L:349:PRO:HG3	2.48	0.49
1:K:145:PHE:N	1:K:145:PHE:CD1	2.80	0.49
1:I:123:ALA:HB3	1:I:144:TYR:HE2	1.78	0.48
2:J:360:ASP:OD2	2:J:428:ARG:HD2	2.14	0.48
2:H:390:LYS:HD2	5:H:3677:HOH:O	2.13	0.48
1:C:98:THR:H	1:C:101:ALA:HB3	1.78	0.48
2:J:449:TRP:CD1	2:J:457:ARG:HG2	2.49	0.48
2:F:381:ALA:O	2:F:522:ARG:HA	2.14	0.48
1:G:25:ALA:HB1	1:G:98:THR:HG21	1.96	0.48
2:L:410:HIS:HA	2:L:411:LYS:NZ	2.29	0.47
1:K:71:TRP:CD1	2:L:470:ILE:HD13	2.49	0.47
1:G:132:ALA:HB3	1:G:135:ILE:HD12	1.95	0.47
1:I:98:THR:N	1:I:101:ALA:O	2.44	0.47
2:J:484:PRO:O	2:J:487:PRO:HD2	2.14	0.47
2:D:376:GLU:OE1	5:D:1665:HOH:O	2.20	0.47
1:E:15:PRO:HD3	4:F:2550:DHB:C2	2.45	0.47
1:E:15:PRO:HD3	4:F:2550:DHB:C1	2.44	0.47
2:F:368:ASN:HD22	2:F:370:GLY:N	2.12	0.47
2:F:356:PHE:CE1	2:F:428:ARG:HD3	2.50	0.47
1:C:198:PHE:HA	2:D:337:VAL:O	2.14	0.47
2:F:383:ARG:HG3	2:F:436:TYR:CE2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:495:ILE:CG2	5:J:4698:HOH:O	2.63	0.47
1:C:190:GLN:HG3	2:D:333:ARG:HG2	1.97	0.47
1:K:84:ASN:O	1:K:90:ASN:ND2	2.39	0.46
1:E:132:ALA:HB3	1:E:135:ILE:HD12	1.96	0.46
2:D:411:LYS:CE	2:D:411:LYS:H	2.28	0.46
2:H:454:ASN:HB2	2:J:310:ILE:HD13	1.97	0.46
2:L:495:ILE:HG21	2:L:500:ALA:HB3	1.98	0.46
2:B:356:PHE:CD1	2:B:428:ARG:HD3	2.50	0.46
1:I:123:ALA:HB3	1:I:144:TYR:CE2	2.50	0.46
2:J:405:GLY:HA3	5:J:4682:HOH:O	2.16	0.46
2:J:363:LEU:N	2:J:363:LEU:HD12	2.31	0.46
2:H:493:LYS:C	2:H:495:ILE:H	2.20	0.46
1:I:92:PHE:CD1	2:J:349:PRO:HG3	2.50	0.46
1:C:67:PHE:CZ	1:C:94:ARG:HD2	2.50	0.46
2:J:363:LEU:HD23	2:J:425:GLY:HA2	1.97	0.46
2:J:411:LYS:H	2:J:411:LYS:NZ	2.15	0.45
2:F:486:ILE:HD13	2:F:486:ILE:HG21	1.76	0.45
2:L:441:THR:OG1	2:L:442:ILE:N	2.50	0.45
1:C:20:GLY:HA2	2:D:426:VAL:HG13	1.97	0.45
2:B:495:ILE:HG21	2:B:500:ALA:HB3	1.98	0.45
2:H:368:ASN:ND2	2:H:371:GLY:H	2.14	0.45
2:L:303:GLN:C	2:L:303:GLN:CB	2.74	0.45
2:D:368:ASN:HD22	2:D:369:ASN:N	2.14	0.45
2:B:419:LEU:HD23	2:B:419:LEU:HA	1.80	0.45
2:D:321:THR:HG21	2:D:494:SER:HB2	1.97	0.45
1:K:50:LEU:O	1:K:182:ALA:HA	2.17	0.45
1:G:15:PRO:HD3	4:H:3550:DHB:C2	2.47	0.45
1:K:174:ARG:HE	1:K:181:THR:CG2	2.29	0.45
2:B:489:CYS:HA	2:B:490:PRO:HD3	1.79	0.45
2:L:447:TYR:CE1	4:L:5550:DHB:H5	2.47	0.45
2:H:411:LYS:HE2	2:H:411:LYS:HB2	1.67	0.45
2:F:458:PRO:HD3	2:F:489:CYS:HB2	1.98	0.45
2:H:411:LYS:HZ3	2:H:411:LYS:H	1.65	0.45
1:E:64:ARG:HG2	1:E:64:ARG:HH11	1.81	0.45
1:G:143:LEU:HD23	1:G:143:LEU:C	2.37	0.45
1:A:39:LEU:HD12	1:A:39:LEU:N	2.31	0.45
1:K:160:LEU:HD23	1:K:160:LEU:HA	1.82	0.45
2:H:368:ASN:HD22	2:H:370:GLY:N	2.10	0.44
2:H:447:TYR:HE1	4:H:3550:DHB:H5	1.82	0.44
2:B:356:PHE:HD1	2:B:428:ARG:HD3	1.80	0.44
1:A:67:PHE:HZ	1:A:94:ARG:HD2	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:92:PHE:CG	2:L:349:PRO:HG3	2.52	0.44
2:D:443:LYS:HG2	2:D:444:PRO:HD2	2.00	0.44
1:I:50:LEU:HD13	1:I:107:HIS:CE1	2.53	0.44
1:I:31:ARG:NH1	2:J:428:ARG:HG2	2.32	0.44
1:I:160:LEU:HA	1:I:160:LEU:HD23	1.56	0.44
2:F:447:TYR:CZ	4:F:2550:DHB:O4	2.70	0.44
2:L:410:HIS:HA	2:L:411:LYS:HZ1	1.83	0.44
1:K:6:PRO:HB2	2:L:503:GLN:HE22	1.83	0.44
2:J:447:TYR:OH	4:J:4550:DHB:O4	2.36	0.44
2:B:522:ARG:NH1	5:B:716:HOH:O	2.51	0.44
2:D:449:TRP:CD1	2:D:449:TRP:N	2.86	0.44
2:L:449:TRP:N	2:L:449:TRP:CD1	2.85	0.44
1:I:67:PHE:CZ	1:I:94:ARG:HD2	2.52	0.44
1:A:50:LEU:O	1:A:182:ALA:HA	2.18	0.44
1:G:35:ILE:HG21	1:G:92:PHE:CE2	2.53	0.44
2:B:403:ASN:HB2	5:B:620:HOH:O	2.17	0.44
1:K:17:VAL:HG22	1:K:21:LEU:HD12	1.99	0.43
1:I:123:ALA:O	1:I:124:PRO:C	2.56	0.43
1:K:50:LEU:HD12	1:K:106:LEU:O	2.17	0.43
1:C:4:LEU:HB2	5:C:3765:HOH:O	2.17	0.43
2:D:497:ASN:C	2:D:497:ASN:HD22	2.20	0.43
1:K:9:PRO:HG2	2:L:500:ALA:HB1	2.00	0.43
2:D:465:ILE:N	2:D:465:ILE:HD13	2.34	0.43
1:E:5:LEU:O	2:F:387:GLN:HG2	2.19	0.43
2:B:447:TYR:CE1	4:B:550:DHB:H5	2.54	0.43
1:G:163:GLN:HA	1:G:164:PRO:HD2	1.97	0.43
1:E:52:LEU:C	1:E:52:LEU:HD22	2.38	0.43
1:K:65:ASP:OD2	1:K:133:ARG:HD3	2.19	0.43
1:A:132:ALA:HB3	1:A:135:ILE:HD12	1.99	0.43
2:L:400:TRP:HA	2:L:425:GLY:O	2.18	0.43
2:B:411:LYS:HE2	2:B:411:LYS:HB2	1.70	0.43
2:J:465:ILE:HD12	2:J:465:ILE:N	2.34	0.43
2:J:497:ASN:HA	2:J:498:PRO:HD2	1.88	0.43
1:I:144:TYR:CE1	1:I:158:LEU:HD13	2.53	0.43
2:D:396:LEU:HA	2:D:396:LEU:HD12	1.75	0.43
1:C:85:LEU:HA	1:C:85:LEU:HD23	1.57	0.43
2:J:336:LEU:HD23	2:J:336:LEU:HA	1.70	0.43
2:B:316:HIS:HB3	2:B:317:PRO:HD2	2.01	0.43
2:B:418:PRO:HG2	2:H:374:ILE:HD13	1.99	0.43
2:D:408[B]:CYS:CA	2:D:408[B]:CYS:SG	3.03	0.43
2:L:361:HIS:HD2	2:L:361:HIS:H	1.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:399:MET:HA	2:F:462:HIS:O	2.18	0.43
2:H:307:ARG:HG2	2:H:533:THR:HG22	2.01	0.43
1:K:19:ILE:HG21	2:L:410:HIS:HB2	2.00	0.42
1:G:125:HIS:HA	1:G:143:LEU:O	2.19	0.42
2:B:447:TYR:HE1	4:B:550:DHB:H5	1.84	0.42
2:H:419:LEU:HA	2:H:419:LEU:HD23	1.83	0.42
1:I:4:LEU:HB3	2:J:387:GLN:HB3	2.00	0.42
2:B:449:TRP:CH2	2:B:491:ILE:HD12	2.55	0.42
1:E:77:GLY:O	1:E:114:VAL:HG12	2.19	0.42
1:E:7:GLU:OE2	2:F:311:ARG:HG2	2.20	0.42
2:H:511:ASN:ND2	2:H:511:ASN:H	2.16	0.42
2:J:350:ASN:C	2:J:350:ASN:OD1	2.58	0.42
2:H:522:ARG:NH1	5:H:3716:HOH:O	2.52	0.42
2:J:393:PRO:O	2:J:394:ASN:C	2.57	0.42
2:L:306:SER:HB2	5:L:5818:HOH:O	2.18	0.42
1:E:170:LEU:HD21	1:E:196:VAL:HB	2.02	0.42
2:D:411:LYS:HE2	2:D:411:LYS:HB2	1.64	0.42
1:A:98:THR:N	1:A:101:ALA:O	2.53	0.42
1:I:92:PHE:CG	2:J:349:PRO:HG3	2.54	0.42
1:C:163:GLN:HA	1:C:164:PRO:HD2	1.81	0.42
2:B:305:ASN:O	2:B:533:THR:HG23	2.19	0.42
2:F:315:TRP:HZ2	2:F:503:GLN:HE21	1.68	0.42
2:D:307:ARG:HD3	2:D:307:ARG:HA	1.82	0.42
1:K:19:ILE:CG2	2:L:410:HIS:HB2	2.50	0.41
1:A:78:GLU:OE1	2:B:301:PRO:HG3	2.20	0.41
1:C:18:HIS:CB	1:C:26:ALA:HB2	2.50	0.41
1:A:67:PHE:CZ	1:A:94:ARG:HD2	2.55	0.41
2:F:488:MET:O	2:F:490:PRO:HD3	2.19	0.41
1:G:18:HIS:HB2	1:G:26:ALA:HB2	2.02	0.41
1:K:123:ALA:HB3	1:K:144:TYR:CE2	2.55	0.41
1:K:85:LEU:HD23	1:K:85:LEU:HA	1.49	0.41
1:E:52:LEU:HD23	1:E:103:GLU:HG2	2.02	0.41
1:E:123:ALA:O	1:E:124:PRO:C	2.57	0.41
1:E:68:LEU:N	1:E:68:LEU:HD12	2.35	0.41
1:K:158:LEU:HA	1:K:158:LEU:HD12	1.80	0.41
2:J:356:PHE:CD1	2:J:428:ARG:HD3	2.56	0.41
2:D:497:ASN:HD22	2:D:498:PRO:N	2.18	0.41
2:B:307:ARG:HG2	2:B:533:THR:HG22	2.03	0.41
1:K:170:LEU:HA	1:K:170:LEU:HD23	1.65	0.41
2:J:475:ILE:HD13	2:J:475:ILE:HG21	1.72	0.41
2:B:489:CYS:SG	2:B:489:CYS:CA	2.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:HIS:ND1	1:E:163:GLN:HG3	2.35	0.41
1:A:163:GLN:HA	1:A:164:PRO:HD2	1.78	0.41
2:L:457:ARG:HH11	2:L:457:ARG:HD3	1.70	0.41
2:D:411:LYS:HZ3	2:D:411:LYS:H	1.69	0.41
2:F:356:PHE:HD1	2:F:428:ARG:CD	2.33	0.41
1:E:92:PHE:CG	2:F:349:PRO:HG3	2.56	0.41
2:F:356:PHE:HD1	2:F:428:ARG:HD3	1.84	0.41
1:E:123:ALA:HB3	1:E:144:TYR:HE2	1.86	0.41
1:K:72:GLN:O	1:K:72:GLN:HG3	2.21	0.41
2:D:412:ASN:HD22	2:D:412:ASN:HA	1.68	0.41
2:L:304:ASP:OD1	2:L:307:ARG:NH1	2.41	0.41
2:B:354:LEU:HD12	2:B:354:LEU:HA	1.77	0.41
1:I:85:LEU:HA	1:I:85:LEU:HD23	1.71	0.41
1:E:63:VAL:HG12	1:E:66:SER:HB3	2.02	0.41
1:K:146:ASP:OD1	1:K:174:ARG:HB2	2.21	0.40
1:G:35:ILE:HG21	1:G:92:PHE:HE2	1.87	0.40
2:F:411:LYS:NZ	2:F:411:LYS:H	2.19	0.40
2:L:307:ARG:HA	2:L:307:ARG:HD3	1.63	0.40
2:B:390:LYS:HA	2:B:391:PRO:HD3	1.88	0.40
2:F:411:LYS:HE2	2:F:411:LYS:HB2	1.77	0.40
1:C:94:ARG:NH2	2:D:398:GLU:OE2	2.54	0.40
2:B:315:TRP:CZ2	2:B:503:GLN:NE2	2.89	0.40
1:G:18:HIS:CB	1:G:26:ALA:HB2	2.51	0.40
2:F:480:PHE:O	2:F:481:GLU:C	2.59	0.40
1:A:85:LEU:HA	1:A:85:LEU:HD23	1.90	0.40
2:F:493:LYS:HE2	2:F:493:LYS:HB2	1.89	0.40
1:E:65:ASP:OD2	1:E:133:ARG:HD3	2.21	0.40
1:C:94:ARG:HH22	2:D:398:GLU:CD	2.24	0.40
1:A:110:LYS:NZ	1:A:147:ASP:OD1	2.55	0.40
1:E:31:ARG:NH1	2:F:428:ARG:HG2	2.36	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:538:CYS:OXT	5:D:1833:HOH:O[2_555]	1.83	0.37
2:L:538:CYS:OXT	5:J:4833:HOH:O[2_555]	1.93	0.27
2:H:538:CYS:OXT	5:F:2833:HOH:O[2_555]	2.01	0.19
2:B:538:CYS:OXT	5:L:5833:HOH:O[2_555]	2.03	0.17

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%)	189 (96%)	9 (4%)	0	100	100
1	C	198/200 (99%)	189 (96%)	9 (4%)	0	100	100
1	E	198/200 (99%)	188 (95%)	10 (5%)	0	100	100
1	G	198/200 (99%)	188 (95%)	10 (5%)	0	100	100
1	I	198/200 (99%)	183 (92%)	15 (8%)	0	100	100
1	K	198/200 (99%)	180 (91%)	17 (9%)	1 (0%)	34	34
2	B	237/238 (100%)	227 (96%)	9 (4%)	1 (0%)	39	43
2	D	237/238 (100%)	222 (94%)	14 (6%)	1 (0%)	39	43
2	F	237/238 (100%)	229 (97%)	7 (3%)	1 (0%)	39	43
2	H	237/238 (100%)	225 (95%)	11 (5%)	1 (0%)	39	43
2	J	237/238 (100%)	227 (96%)	8 (3%)	2 (1%)	24	21
2	L	237/238 (100%)	221 (93%)	14 (6%)	2 (1%)	24	21
All	All	2610/2628 (99%)	2468 (95%)	133 (5%)	9 (0%)	46	52

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	368	ASN
2	D	368	ASN
2	F	368	ASN
2	H	368	ASN
2	J	368	ASN
2	L	368	ASN
2	L	369	ASN
1	K	179	GLY
2	J	394	ASN

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%)	152 (94%)	10 (6%)	23 22
1	C	162/163 (99%)	148 (91%)	14 (9%)	13 11
1	E	162/163 (99%)	149 (92%)	13 (8%)	15 13
1	G	162/163 (99%)	153 (94%)	9 (6%)	26 27
1	I	162/163 (99%)	148 (91%)	14 (9%)	13 11
1	K	162/163 (99%)	146 (90%)	16 (10%)	10 7
2	B	201/202 (100%)	179 (89%)	22 (11%)	8 6
2	D	201/202 (100%)	181 (90%)	20 (10%)	9 7
2	F	201/202 (100%)	184 (92%)	17 (8%)	13 11
2	H	201/202 (100%)	179 (89%)	22 (11%)	8 6
2	J	201/202 (100%)	182 (90%)	19 (10%)	11 8
2	L	201/202 (100%)	182 (90%)	19 (10%)	11 8
All	All	2178/2190 (100%)	1983 (91%)	195 (9%)	12 10

All (195) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ILE
1	A	4	LEU
1	A	38	ARG
1	A	52	LEU
1	A	68	LEU
1	A	94	ARG
1	A	106	LEU
1	A	133	ARG
1	A	165	GLN
1	A	192	GLU
2	B	301	PRO
2	B	320	LEU
2	B	327	SER
2	B	364	LEU

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Mol	Chain	Res	Type
2	B	368	ASN
2	B	372	LEU
2	B	395	THR
2	B	399	MET
2	B	411	LYS
2	B	414	ARG
2	B	416	LEU
2	B	428	ARG
2	B	434	ASP
2	B	443	LYS
2	B	473	LYS
2	B	474	LEU
2	B	491	ILE
2	B	497	ASN
2	B	507	LYS
2	B	534	HIS
2	B	537	ASN
2	B	538	CYS
1	C	4	LEU
1	C	32	ASP
1	C	38	ARG
1	C	41	LYS
1	C	42	PRO
1	C	52	LEU
1	C	91	SER
1	C	94	ARG
1	C	150	GLN
1	C	154	LYS
1	C	158	LEU
1	C	165	GLN
1	C	180	LYS
1	C	188	ARG
2	D	306	SER
2	D	364	LEU
2	D	372	LEU
2	D	391	PRO
2	D	393	PRO
2	D	395	THR
2	D	399	MET
2	D	411	LYS
2	D	428	ARG
2	D	433	SER

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Mol	Chain	Res	Type
2	D	448	PRO
2	D	450	ARG
2	D	457	ARG
2	D	465	ILE
2	D	493	LYS
2	D	497	ASN
2	D	499	GLU
2	D	515	PRO
2	D	534	HIS
2	D	537	ASN
1	E	2	ILE
1	E	4	LEU
1	E	19	ILE
1	E	49	ILE
1	E	52	LEU
1	E	91	SER
1	E	98	THR
1	E	158	LEU
1	E	164	PRO
1	E	165	GLN
1	E	180	LYS
1	E	181	THR
1	E	188	ARG
2	F	324	TYR
2	F	364	LEU
2	F	368	ASN
2	F	372	LEU
2	F	393	PRO
2	F	395	THR
2	F	411	LYS
2	F	416	LEU
2	F	428	ARG
2	F	434	ASP
2	F	442	ILE
2	F	450	ARG
2	F	497	ASN
2	F	499	GLU
2	F	507	LYS
2	F	534	HIS
2	F	538	CYS
1	G	4	LEU
1	G	19	ILE

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Mol	Chain	Res	Type
1	G	38	ARG
1	G	52	LEU
1	G	91	SER
1	G	94	ARG
1	G	133	ARG
1	G	154	LYS
1	G	165	GLN
2	H	306	SER
2	H	344	SER
2	H	364	LEU
2	H	372	LEU
2	H	394	ASN
2	H	395	THR
2	H	411	LYS
2	H	414	ARG
2	H	416	LEU
2	H	428	ARG
2	H	433	SER
2	H	434	ASP
2	H	442	ILE
2	H	449	TRP
2	H	465	ILE
2	H	470	ILE
2	H	473	LYS
2	H	497	ASN
2	H	503	GLN
2	H	507	LYS
2	H	511	ASN
2	H	534	HIS
1	I	2	ILE
1	I	4	LEU
1	I	38	ARG
1	I	42	PRO
1	I	49	ILE
1	I	52	LEU
1	I	66	SER
1	I	124	PRO
1	I	133	ARG
1	I	146	ASP
1	I	150	GLN
1	I	165	GLN
1	I	168	GLU

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Mol	Chain	Res	Type
1	I	180	LYS
2	J	306	SER
2	J	364	LEU
2	J	372	LEU
2	J	394	ASN
2	J	395	THR
2	J	399	MET
2	J	411	LYS
2	J	416	LEU
2	J	428	ARG
2	J	442	ILE
2	J	450	ARG
2	J	457	ARG
2	J	473	LYS
2	J	495	ILE
2	J	497	ASN
2	J	499	GLU
2	J	507	LYS
2	J	534	HIS
2	J	538	CYS
1	K	4	LEU
1	K	9	PRO
1	K	21	LEU
1	K	30	THR
1	K	52	LEU
1	K	68	LEU
1	K	78	GLU
1	K	91	SER
1	K	94	ARG
1	K	100	ASP
1	K	143	LEU
1	K	158	LEU
1	K	165	GLN
1	K	178	ASP
1	K	181	THR
1	K	188	ARG
2	L	328	ILE
2	L	364	LEU
2	L	368	ASN
2	L	372	LEU
2	L	401	GLN
2	L	411	LYS

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Mol	Chain	Res	Type
2	L	414	ARG
2	L	416	LEU
2	L	428	ARG
2	L	434	ASP
2	L	450	ARG
2	L	457	ARG
2	L	473	LYS
2	L	478	LEU
2	L	497	ASN
2	L	507	LYS
2	L	515	PRO
2	L	534	HIS
2	L	538	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	61	HIS
1	A	163	GLN
1	A	165	GLN
2	B	361	HIS
2	B	368	ASN
2	B	369	ASN
2	B	412	ASN
2	B	497	ASN
2	B	503	GLN
1	C	107	HIS
1	C	165	GLN
2	D	361	HIS
2	D	368	ASN
2	D	412	ASN
2	D	497	ASN
2	D	503	GLN
1	E	165	GLN
2	F	361	HIS
2	F	368	ASN
2	F	497	ASN
2	F	503	GLN
2	F	511	ASN
1	G	165	GLN
2	H	361	HIS

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Mol	Chain	Res	Type
2	H	368	ASN
2	H	412	ASN
2	H	497	ASN
2	H	503	GLN
1	I	107	HIS
1	I	127	ASN
1	I	165	GLN
2	J	361	HIS
2	J	368	ASN
2	J	412	ASN
2	J	422	ASN
2	J	497	ASN
2	J	503	GLN
2	J	530	GLN
1	K	165	GLN
2	L	361	HIS
2	L	368	ASN
2	L	369	ASN
2	L	412	ASN
2	L	422	ASN
2	L	497	ASN
2	L	503	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 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	DHB	B	550	3,2	8,11,11	0.87	0	11,15,15	0.61	0
4	DHB	D	1550	3	8,11,11	0.74	0	11,15,15	0.66	0
4	DHB	F	2550	3	8,11,11	1.48	2 (25%)	11,15,15	1.26	2 (18%)
4	DHB	H	3550	3	8,11,11	0.59	0	11,15,15	0.69	0
4	DHB	J	4550	-	8,11,11	0.64	0	11,15,15	0.85	0
4	DHB	L	5550	3	8,11,11	0.51	0	11,15,15	0.76	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	DHB	B	550	3,2	-	0/0/4/4	0/1/1/1
4	DHB	D	1550	3	-	0/0/4/4	0/1/1/1
4	DHB	F	2550	3	-	0/0/4/4	0/1/1/1
4	DHB	H	3550	3	-	0/0/4/4	0/1/1/1
4	DHB	J	4550	-	-	0/0/4/4	0/1/1/1
4	DHB	L	5550	3	-	0/0/4/4	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	2550	DHB	C6-C1	-2.60	1.33	1.39
4	F	2550	DHB	C4-C3	2.64	1.44	1.40

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	2550	DHB	C1-C2-C3	-2.16	119.16	120.98
4	F	2550	DHB	C6-C1-C2	2.51	121.50	118.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	550	DHB	3	0
4	D	1550	DHB	2	0
4	F	2550	DHB	5	0
4	H	3550	DHB	3	0
4	J	4550	DHB	3	0
4	L	5550	DHB	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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	200/200 (100%)	-0.53	3 (1%)	76	79	18, 33, 64, 73	0
1	C	200/200 (100%)	-0.48	3 (1%)	76	79	18, 32, 64, 73	0
1	E	200/200 (100%)	-0.38	4 (2%)	68	72	18, 33, 65, 74	0
1	G	200/200 (100%)	-0.39	8 (4%)	42	45	19, 33, 66, 74	0
1	I	200/200 (100%)	-0.39	9 (4%)	37	41	19, 35, 65, 74	0
1	K	200/200 (100%)	-0.30	11 (5%)	29	32	20, 37, 67, 74	0
2	B	238/238 (100%)	-0.65	7 (2%)	55	60	18, 26, 52, 71	0
2	D	238/238 (100%)	-0.65	7 (2%)	55	60	17, 25, 52, 71	0
2	F	238/238 (100%)	-0.70	7 (2%)	55	60	18, 26, 53, 70	0
2	H	238/238 (100%)	-0.70	3 (1%)	79	82	17, 26, 53, 69	0
2	J	238/238 (100%)	-0.69	6 (2%)	61	65	21, 28, 53, 72	0
2	L	238/238 (100%)	-0.68	6 (2%)	61	65	20, 28, 54, 71	0
All	All	2628/2628 (100%)	-0.56	74 (2%)	56	61	17, 30, 60, 74	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	99	PHE	5.8
2	B	301	PRO	5.4
1	I	99	PHE	4.9
1	G	99	PHE	4.5
1	K	99	PHE	4.4
1	G	100	ASP	4.2
1	K	177	VAL	4.1
2	L	301	PRO	4.1
1	C	99	PHE	4.0
1	G	177	VAL	4.0
1	E	100	ASP	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	99	PHE	3.9
2	F	368	ASN	3.9
1	K	178	ASP	3.8
2	J	414	ARG	3.5
1	I	100	ASP	3.5
2	F	370	GLY	3.5
2	L	538	CYS	3.5
2	B	537	ASN	3.4
1	E	177	VAL	3.4
2	L	370	GLY	3.3
2	H	301	PRO	3.3
2	B	368	ASN	3.2
1	C	100	ASP	3.2
2	J	537	ASN	3.2
1	G	178	ASP	3.1
2	D	369	ASN	3.1
2	H	537	ASN	3.1
1	G	176	GLU	3.0
1	K	43	ASP	3.0
1	K	179	GLY	3.0
1	A	178	ASP	3.0
1	I	178	ASP	3.0
2	L	369	ASN	3.0
2	L	537	ASN	3.0
2	F	301	PRO	2.9
1	A	100	ASP	2.8
2	J	369	ASN	2.8
1	I	177	VAL	2.8
2	H	414	ARG	2.8
2	B	414	ARG	2.7
1	G	27	GLY	2.7
2	D	368	ASN	2.6
1	I	25	ALA	2.6
1	K	100	ASP	2.6
2	L	368	ASN	2.6
2	D	411	LYS	2.6
2	F	538	CYS	2.6
1	I	32	ASP	2.5
1	I	24	GLU	2.5
1	I	179	GLY	2.4
2	B	370	GLY	2.4
2	F	305	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
2	F	537	ASN	2.4
2	D	414	ARG	2.3
1	K	30	THR	2.3
1	I	176	GLU	2.3
1	K	86	GLU	2.3
1	G	26	ALA	2.2
2	B	369	ASN	2.2
1	K	32	ASP	2.2
1	K	180	LYS	2.2
2	F	414	ARG	2.2
1	E	26	ALA	2.2
2	J	411	LYS	2.2
1	G	179	GLY	2.1
2	D	301	PRO	2.1
2	J	368	ASN	2.1
2	B	303	GLN	2.1
2	J	305	ASN	2.1
1	C	26	ALA	2.1
2	D	538	CYS	2.1
1	K	176	GLU	2.1
2	D	537	ASN	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	DHB	L	5550	11/11	0.88	0.20	7.58	65,67,68,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	DHB	F	2550	11/11	0.88	0.18	7.08	52,56,58,59	0
4	DHB	J	4550	11/11	0.83	0.21	5.78	66,67,68,68	0
4	DHB	D	1550	11/11	0.88	0.18	5.51	57,59,59,60	0
4	DHB	H	3550	11/11	0.80	0.21	4.52	63,70,72,74	0
4	DHB	B	550	11/11	0.87	0.14	3.82	53,57,59,61	0
3	FE	L	600	1/1	0.97	0.07	-0.76	76,76,76,76	0
3	FE	F	600	1/1	0.88	0.05	-2.12	79,79,79,79	0
3	FE	B	600	1/1	0.99	0.04	-2.64	85,85,85,85	0
3	FE	H	600	1/1	0.95	0.05	-	84,84,84,84	0
3	FE	D	600	1/1	0.92	0.06	-	81,81,81,81	0
3	FE	J	600	1/1	0.87	0.08	-	93,93,93,93	0

6.5 Other polymers (i)

There are no such residues in this entry.