Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:47 PM GMT

PDB ID	:	1YKP
Title	:	Protocatechuate 3,4-Dioxygenase Y408H mutant bound to DHB
Authors	:	Brown, C.K.; Ohlendorf, D.H.
Deposited on	:	2005-01-18
Resolution	:	2.41 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 ⓘ symbol.

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

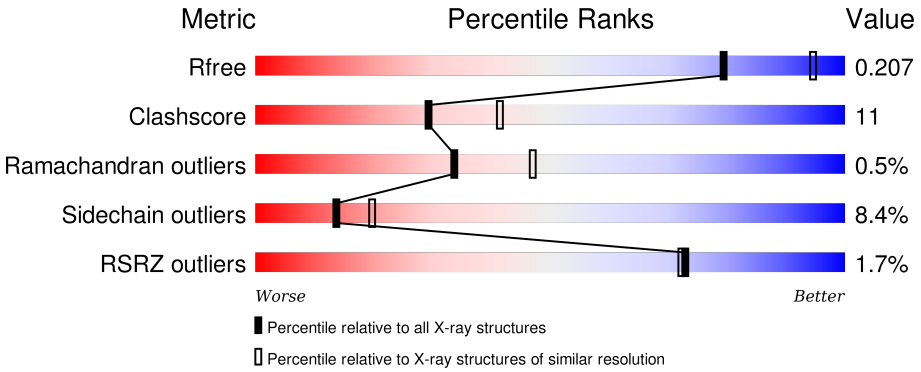
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.41 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	3386 (2.44-2.40)
Clashscore	102246	3897 (2.44-2.40)
Ramachandran outliers	100387	3837 (2.44-2.40)
Sidechain outliers	100360	3838 (2.44-2.40)
RSRZ outliers	91569	3396 (2.44-2.40)

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	54% 35% 11%
1	C	200	47% 43% 8%
1	E	200	47% 42% 10%
1	G	200	56% 31% 10%
1	I	200	51% 41% 7%

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Mol	Chain	Length	Quality of chain
1	K	200	5% 36% 48% 14%
2	B	238	% 51% 34% 14%
2	D	238	2% 49% 39% 10%
2	F	238	% 50% 37% 9%
2	H	238	% 51% 36% 10%
2	J	238	% 48% 35% 13%
2	L	238	2% 47% 37% 15%

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

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 21546 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	0	0
			1877	1187	344	337	9			
2	D	238	Total	C	N	O	S	0	0	0
			1877	1187	344	337	9			
2	F	238	Total	C	N	O	S	0	0	0
			1877	1187	344	337	9			
2	H	238	Total	C	N	O	S	0	0	0
			1877	1187	344	337	9			
2	J	238	Total	C	N	O	S	0	0	0
			1877	1187	344	337	9			
2	L	238	Total	C	N	O	S	0	0	0
			1877	1187	344	337	9			

There are 12 discrepancies between the modelled and reference sequences:

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

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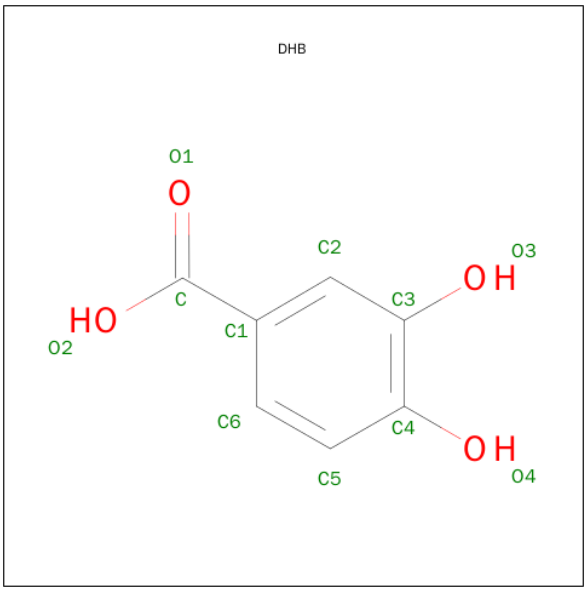
Chain	Residue	Modelled	Actual	Comment	Reference
B	429	CME	CYS	MODIFIED RESIDUE	UNP P00437
D	408	HIS	TYR	ENGINEERED	UNP P00437
D	429	CME	CYS	MODIFIED RESIDUE	UNP P00437
F	408	HIS	TYR	ENGINEERED	UNP P00437
F	429	CME	CYS	MODIFIED RESIDUE	UNP P00437
H	408	HIS	TYR	ENGINEERED	UNP P00437
H	429	CME	CYS	MODIFIED RESIDUE	UNP P00437
J	408	HIS	TYR	ENGINEERED	UNP P00437
J	429	CME	CYS	MODIFIED RESIDUE	UNP P00437
L	408	HIS	TYR	ENGINEERED	UNP P00437
L	429	CME	CYS	MODIFIED RESIDUE	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	A	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	47	Total O 47 47	0	0
5	B	83	Total O 83 83	0	0
5	C	45	Total O 45 45	0	0
5	D	87	Total O 87 87	0	0
5	E	49	Total O 49 49	0	0
5	F	82	Total O 82 82	0	0

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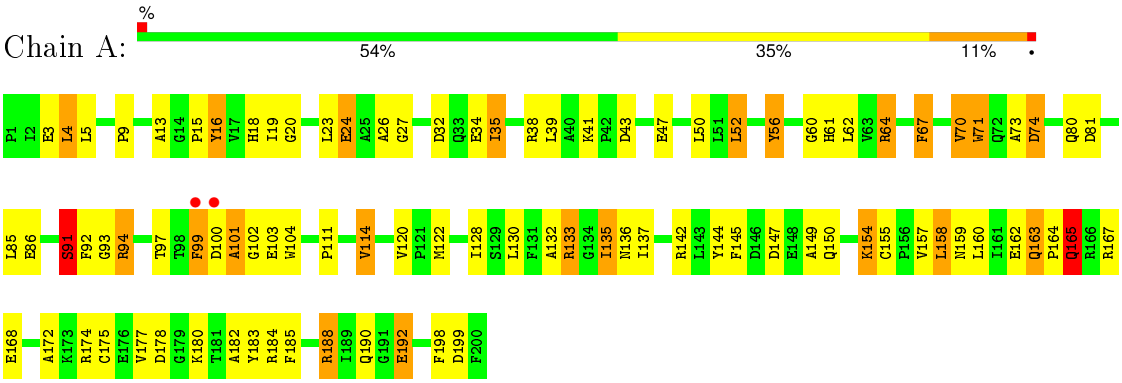
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	G	49	Total O 49 49	0	0
5	H	83	Total O 83 83	0	0
5	I	46	Total O 46 46	0	0
5	J	85	Total O 85 85	0	0
5	K	43	Total O 43 43	0	0
5	L	87	Total O 87 87	0	0

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.

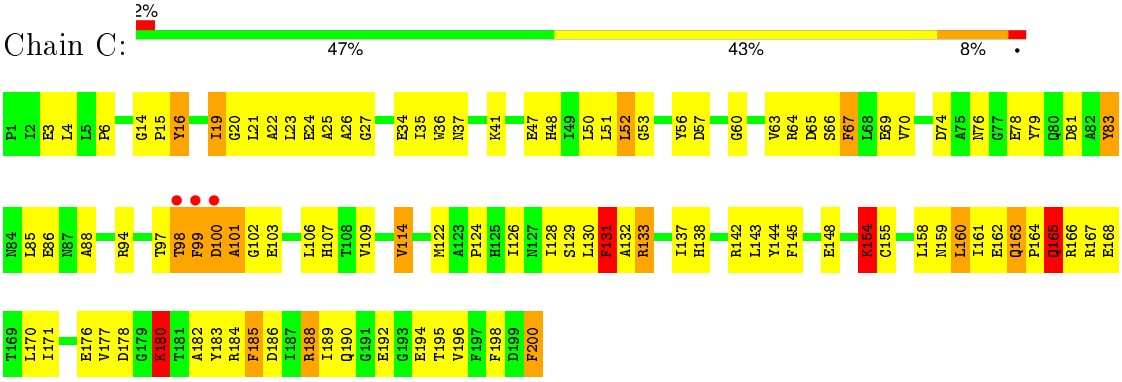
- Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain

Chain A:



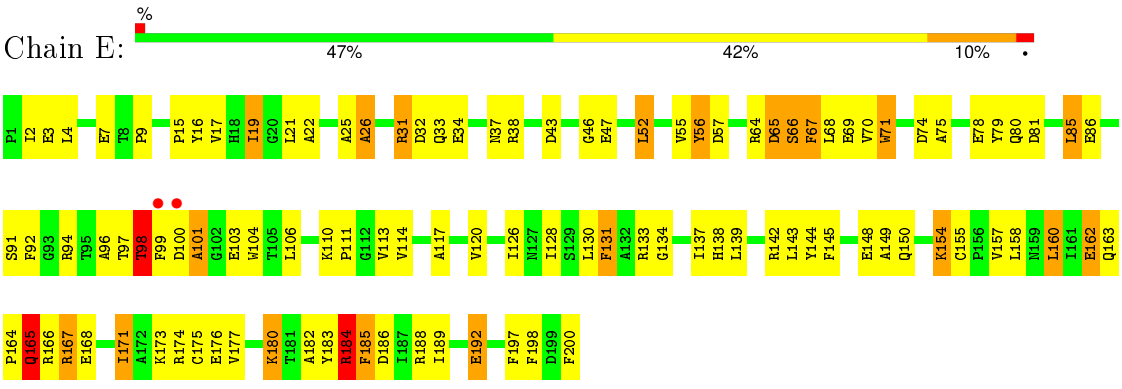
- Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain

Chain C:



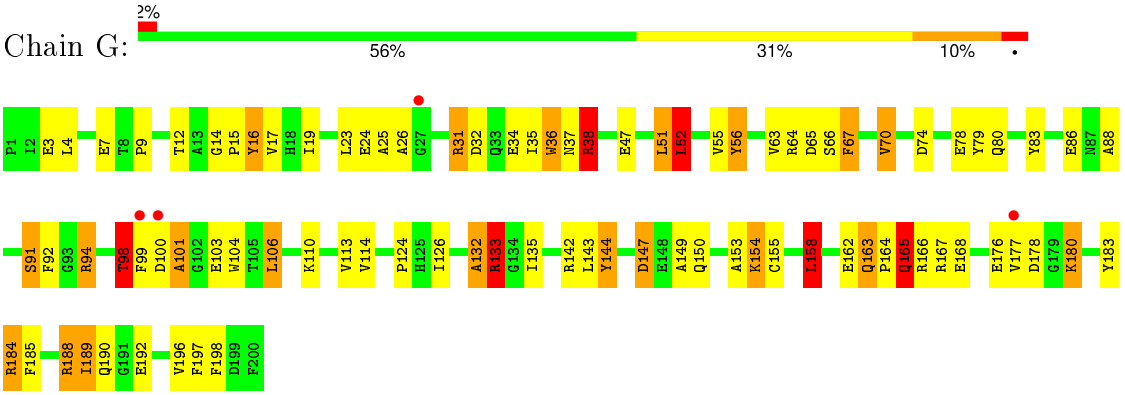
- Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain

Chain E:



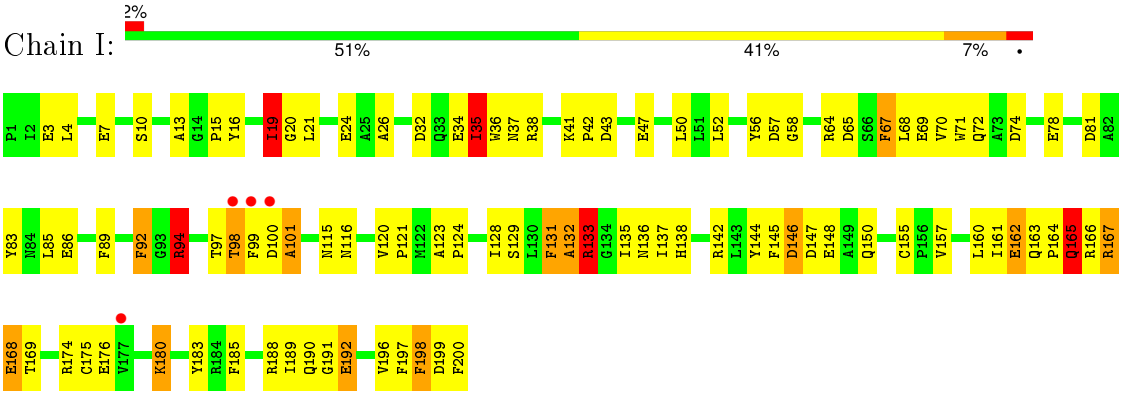
• Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain

Chain G:



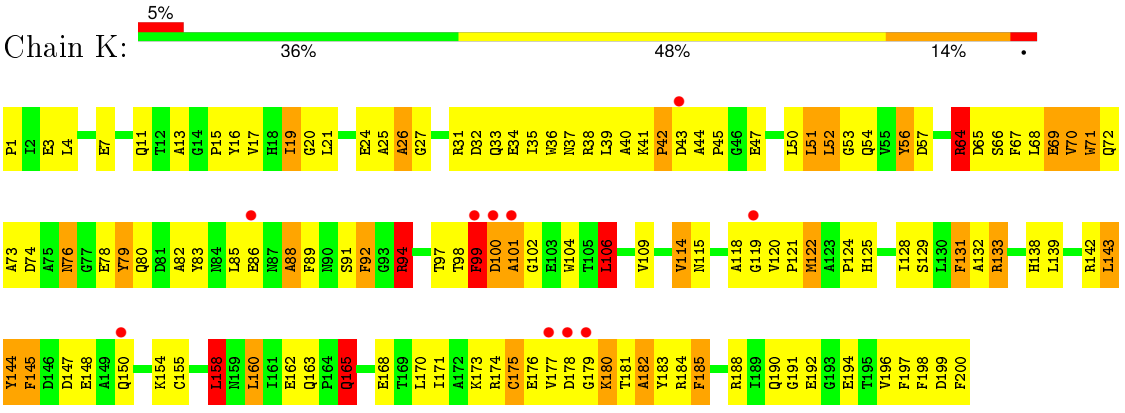
• Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain

Chain I:



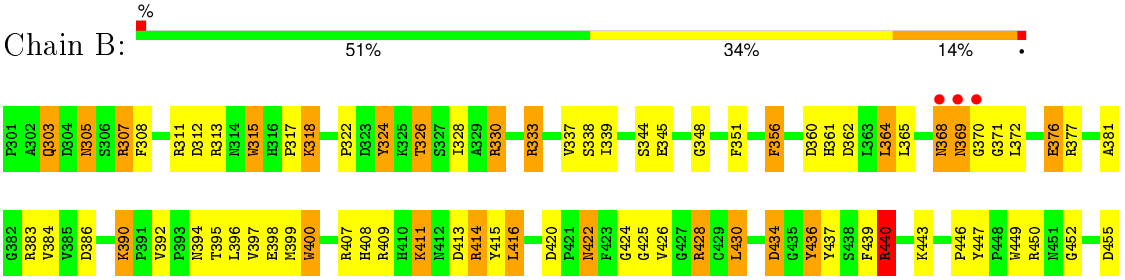
• Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain

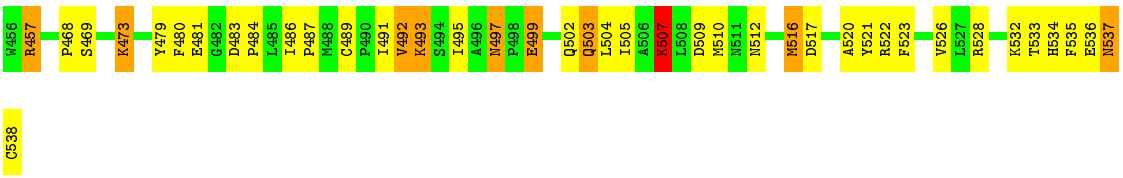
Chain K:



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

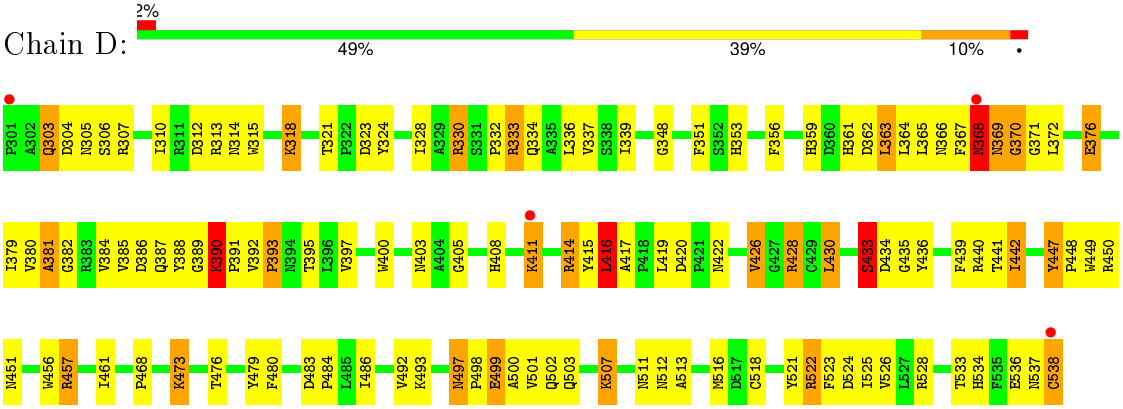
Chain B:





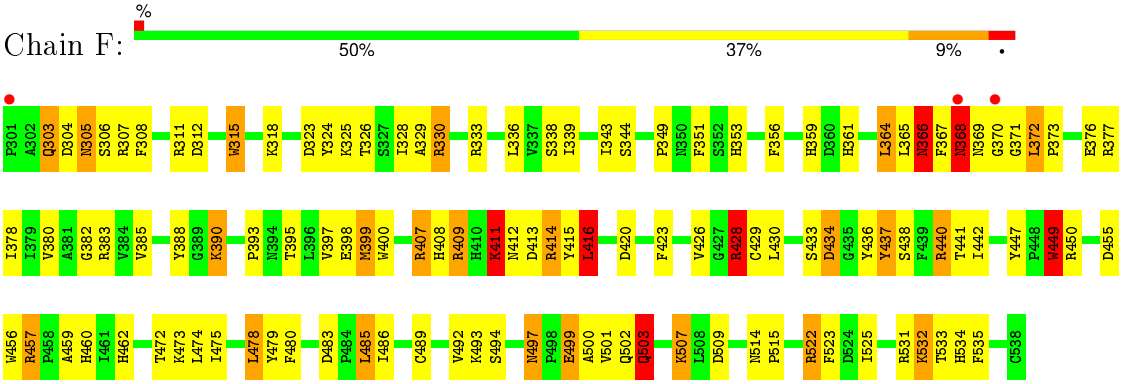
• Molecule 2: Protocatechuate 3,4-dioxygenase beta chain

Chain D:



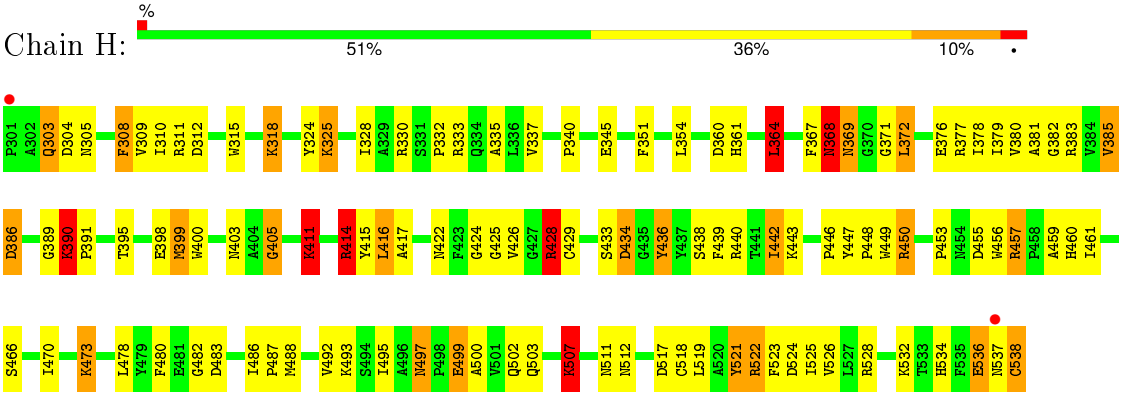
• Molecule 2: Protocatechuate 3,4-dioxygenase beta chain

Chain F:



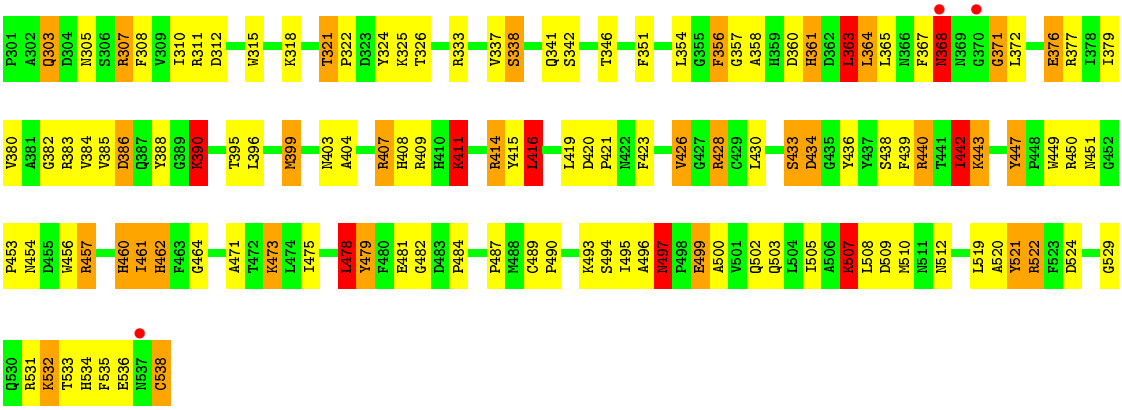
• Molecule 2: Protocatechuate 3,4-dioxygenase beta chain

Chain H:



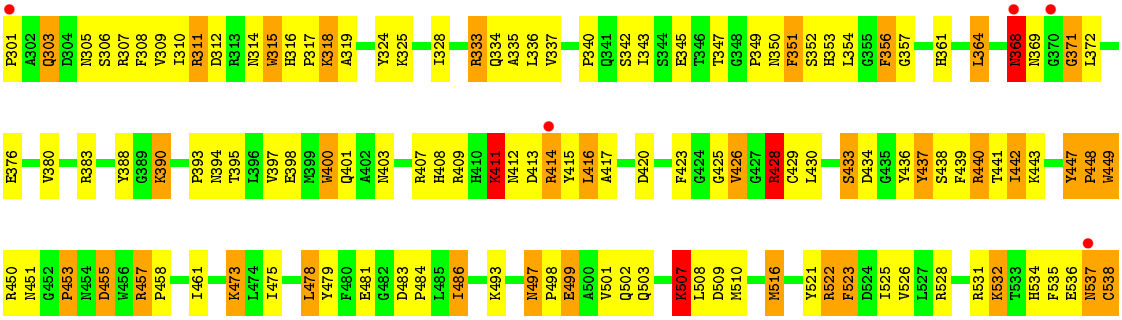
• Molecule 2: Protocatechuate 3,4-dioxygenase beta chain

Chain J:



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

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	196.19Å 127.97Å 134.18Å 90.00° 97.68° 90.00°	Depositor
Resolution (Å)	30.37 – 2.41 30.37 – 1.95	Depositor EDS
% Data completeness (in resolution range)	72.4 (30.37-2.41) 72.5 (30.37-1.95)	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}	0.145 , 0.211 0.144 , 0.207	Depositor DCC
R_{free} test set	1209 reflections (1.33%)	DCC
Wilson B-factor (Å^2)	23.6	Xtriage
Anisotropy	0.420	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 35.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 190284 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	21546	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% 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: CME, 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	2.51	85/1611 (5.3%)	1.92	41/2195 (1.9%)
1	C	2.54	101/1611 (6.3%)	2.13	53/2195 (2.4%)
1	E	2.62	114/1611 (7.1%)	1.96	51/2195 (2.3%)
1	G	2.63	102/1611 (6.3%)	1.93	40/2195 (1.8%)
1	I	2.62	98/1611 (6.1%)	1.98	39/2195 (1.8%)
1	K	2.85	136/1611 (8.4%)	1.98	44/2195 (2.0%)
2	B	2.40	81/1922 (4.2%)	2.02	55/2615 (2.1%)
2	D	2.46	96/1922 (5.0%)	1.97	53/2615 (2.0%)
2	F	2.41	98/1922 (5.1%)	2.02	45/2615 (1.7%)
2	H	2.38	82/1922 (4.3%)	1.98	60/2615 (2.3%)
2	J	2.52	102/1922 (5.3%)	1.93	59/2615 (2.3%)
2	L	2.64	112/1922 (5.8%)	1.93	52/2615 (2.0%)
All	All	2.55	1207/21198 (5.7%)	1.98	592/28860 (2.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	C	0	7
1	E	0	5
1	G	0	6
1	I	0	4
1	K	0	9
2	B	0	9
2	D	0	6
2	F	0	6
2	H	0	5
2	J	0	8

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	L	0	6
All	All	0	75

All (1207) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	532	LYS	CA-CB	16.40	1.90	1.53
2	L	324	TYR	CD1-CE1	16.37	1.64	1.39
1	K	47	GLU	CD-OE2	16.05	1.43	1.25
2	L	426	VAL	CB-CG2	-15.90	1.19	1.52
2	L	436	TYR	CD2-CE2	15.03	1.61	1.39
2	J	538	CYS	CB-SG	-14.77	1.57	1.82
1	K	47	GLU	CD-OE1	14.76	1.41	1.25
1	K	78	GLU	CD-OE1	14.69	1.41	1.25
2	D	376	GLU	CD-OE2	14.35	1.41	1.25
2	H	507	LYS	CE-NZ	14.34	1.84	1.49
2	L	538	CYS	CB-SG	-14.08	1.58	1.82
2	H	303	GLN	CA-CB	13.96	1.84	1.53
1	I	192	GLU	CD-OE2	13.77	1.40	1.25
1	I	47	GLU	CD-OE2	13.57	1.40	1.25
2	B	499	GLU	CD-OE1	13.50	1.40	1.25
1	I	185	PHE	CE2-CZ	13.29	1.62	1.37
1	K	175	CYS	CB-SG	13.06	2.04	1.82
2	J	303	GLN	CA-CB	12.98	1.82	1.53
2	B	303	GLN	CA-CB	12.96	1.82	1.53
1	K	121	PRO	C-O	12.53	1.48	1.23
1	I	183	TYR	CE1-CZ	12.45	1.54	1.38
2	D	426	VAL	CB-CG2	-12.37	1.26	1.52
2	L	499	GLU	CD-OE1	12.27	1.39	1.25
1	A	101	ALA	CA-CB	12.14	1.77	1.52
2	D	303	GLN	CA-CB	12.10	1.80	1.53
1	A	168	GLU	CD-OE1	12.10	1.39	1.25
1	A	47	GLU	CD-OE1	12.09	1.39	1.25
2	J	388	TYR	CD1-CE1	12.05	1.57	1.39
2	F	303	GLN	CA-CB	11.96	1.80	1.53
2	D	507	LYS	CE-NZ	11.95	1.78	1.49
2	F	499	GLU	CD-OE1	11.89	1.38	1.25
2	H	436	TYR	CD1-CE1	11.86	1.57	1.39
1	K	16	TYR	CE2-CZ	11.85	1.53	1.38
1	A	47	GLU	CD-OE2	11.76	1.38	1.25
1	A	114	VAL	CB-CG2	-11.63	1.28	1.52
1	G	47	GLU	CD-OE2	11.61	1.38	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	449	TRP	CZ3-CH2	11.59	1.58	1.40
2	L	303	GLN	CA-CB	11.58	1.79	1.53
2	B	376	GLU	CD-OE2	11.56	1.38	1.25
1	A	86	GLU	CD-OE1	11.55	1.38	1.25
2	L	507	LYS	CE-NZ	11.53	1.77	1.49
1	A	162	GLU	CD-OE1	11.38	1.38	1.25
1	I	47	GLU	CD-OE1	11.28	1.38	1.25
2	H	381	ALA	CA-CB	-11.28	1.28	1.52
1	C	192	GLU	CG-CD	11.25	1.68	1.51
2	L	436	TYR	CD1-CE1	11.22	1.56	1.39
1	C	86	GLU	CD-OE1	11.20	1.38	1.25
1	C	100	ASP	CB-CG	11.19	1.75	1.51
1	G	99	PHE	CD2-CE2	11.19	1.61	1.39
1	K	168	GLU	CD-OE1	11.18	1.38	1.25
1	K	162	GLU	CG-CD	11.15	1.68	1.51
2	J	376	GLU	CD-OE2	11.11	1.37	1.25
2	L	376	GLU	CD-OE2	11.11	1.37	1.25
2	H	436	TYR	CD2-CE2	11.03	1.55	1.39
1	K	86	GLU	CD-OE1	11.02	1.37	1.25
1	K	197	PHE	CE1-CZ	10.97	1.58	1.37
1	G	154	LYS	CD-CE	10.89	1.78	1.51
2	D	376	GLU	CD-OE1	10.80	1.37	1.25
2	B	507	LYS	CD-CE	10.78	1.78	1.51
2	J	426	VAL	CB-CG1	10.77	1.75	1.52
1	C	47	GLU	CD-OE2	10.70	1.37	1.25
1	E	168	GLU	CD-OE1	10.62	1.37	1.25
1	K	78	GLU	CG-CD	10.62	1.67	1.51
2	J	390	LYS	CD-CE	10.57	1.77	1.51
1	C	24	GLU	CD-OE2	10.56	1.37	1.25
2	D	436	TYR	CD1-CE1	10.54	1.55	1.39
2	F	535	PHE	CE2-CZ	10.52	1.57	1.37
1	G	176	GLU	CD-OE1	10.50	1.37	1.25
1	K	78	GLU	CD-OE2	10.49	1.37	1.25
2	L	439	PHE	CE2-CZ	10.46	1.57	1.37
1	G	99	PHE	CD1-CE1	10.42	1.60	1.39
1	E	149	ALA	CA-CB	-10.41	1.30	1.52
1	A	163	GLN	CG-CD	10.37	1.75	1.51
1	K	183	TYR	CE1-CZ	10.34	1.51	1.38
2	D	333	ARG	CZ-NH2	10.31	1.46	1.33
2	D	390	LYS	CD-CE	10.30	1.77	1.51
1	E	192	GLU	CG-CD	10.30	1.67	1.51
2	J	388	TYR	CZ-OH	10.29	1.55	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	162	GLU	CG-CD	10.27	1.67	1.51
1	E	154	LYS	CD-CE	10.25	1.76	1.51
1	K	64	ARG	CZ-NH1	10.24	1.46	1.33
2	F	532	LYS	CA-CB	10.23	1.76	1.53
2	L	376	GLU	CG-CD	10.19	1.67	1.51
1	C	162	GLU	CD-OE2	10.17	1.36	1.25
2	J	532	LYS	CA-CB	10.14	1.76	1.53
2	D	436	TYR	CD2-CE2	10.14	1.54	1.39
2	J	507	LYS	CD-CE	10.12	1.76	1.51
1	A	120	VAL	CB-CG2	-10.10	1.31	1.52
1	G	168	GLU	CD-OE1	10.10	1.36	1.25
2	L	351	PHE	CD2-CE2	10.10	1.59	1.39
1	G	176	GLU	CD-OE2	10.08	1.36	1.25
1	C	192	GLU	CD-OE2	10.04	1.36	1.25
1	C	168	GLU	CD-OE1	10.03	1.36	1.25
1	C	47	GLU	CD-OE1	9.97	1.36	1.25
1	E	176	GLU	CD-OE2	9.94	1.36	1.25
1	E	197	PHE	CD2-CE2	9.93	1.59	1.39
1	G	192	GLU	CD-OE2	9.93	1.36	1.25
1	K	163	GLN	CG-CD	9.93	1.73	1.51
2	H	405	GLY	C-O	9.90	1.39	1.23
1	C	162	GLU	CD-OE1	9.88	1.36	1.25
1	I	16	TYR	CE1-CZ	9.88	1.51	1.38
1	G	16	TYR	CE1-CZ	9.86	1.51	1.38
1	E	56	TYR	CD2-CE2	9.84	1.54	1.39
2	F	426	VAL	CB-CG2	-9.84	1.32	1.52
2	B	318	LYS	CE-NZ	9.84	1.73	1.49
1	E	99	PHE	CD1-CE1	9.83	1.58	1.39
2	J	447	TYR	CE1-CZ	9.81	1.51	1.38
2	B	390	LYS	CD-CE	9.81	1.75	1.51
1	E	154	LYS	CE-NZ	9.79	1.73	1.49
1	I	168	GLU	CD-OE1	9.73	1.36	1.25
2	F	507	LYS	CD-CE	9.73	1.75	1.51
1	G	67	PHE	CE2-CZ	9.71	1.55	1.37
1	G	55	VAL	CB-CG1	-9.68	1.32	1.52
1	E	79	TYR	CD1-CE1	-9.67	1.24	1.39
1	K	16	TYR	CD2-CE2	9.66	1.53	1.39
1	C	183	TYR	CE1-CZ	9.66	1.51	1.38
1	E	7	GLU	CD-OE1	9.65	1.36	1.25
2	F	480	PHE	CD2-CE2	9.59	1.58	1.39
1	C	16	TYR	CE2-CZ	9.55	1.50	1.38
2	L	333	ARG	CZ-NH1	9.50	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	86	GLU	CD-OE1	9.38	1.35	1.25
2	F	376	GLU	CD-OE2	9.36	1.35	1.25
1	I	176	GLU	CD-OE1	9.34	1.35	1.25
1	E	165	GLN	CG-CD	9.32	1.72	1.51
2	F	390	LYS	CD-CE	9.31	1.74	1.51
1	C	188	ARG	CZ-NH1	9.31	1.45	1.33
2	H	415	TYR	CD2-CE2	9.28	1.53	1.39
1	K	165	GLN	CG-CD	9.28	1.72	1.51
2	D	392	VAL	CB-CG1	-9.27	1.33	1.52
2	L	436	TYR	CE1-CZ	9.26	1.50	1.38
1	I	198	PHE	CD1-CE1	9.25	1.57	1.39
1	G	103	GLU	CD-OE2	9.19	1.35	1.25
1	K	16	TYR	CD1-CE1	9.10	1.53	1.39
2	D	507	LYS	CD-CE	9.04	1.73	1.51
1	C	198	PHE	CE2-CZ	9.02	1.54	1.37
2	F	436	TYR	CG-CD1	9.00	1.50	1.39
2	D	538	CYS	CB-SG	-8.95	1.67	1.82
2	D	397	VAL	CB-CG1	-8.94	1.34	1.52
2	D	415	TYR	CD1-CE1	8.94	1.52	1.39
1	I	67	PHE	CE1-CZ	8.94	1.54	1.37
1	I	64	ARG	CZ-NH1	8.93	1.44	1.33
1	A	64	ARG	CZ-NH1	8.93	1.44	1.33
2	J	423	PHE	CE1-CZ	8.92	1.54	1.37
1	E	69	GLU	CB-CG	-8.88	1.35	1.52
1	A	3	GLU	CD-OE1	8.86	1.35	1.25
1	K	3	GLU	CD-OE2	8.84	1.35	1.25
1	E	99	PHE	CE1-CZ	8.82	1.54	1.37
2	H	414	ARG	CB-CG	8.82	1.76	1.52
1	G	99	PHE	CE1-CZ	8.81	1.54	1.37
2	J	436	TYR	CD2-CE2	8.80	1.52	1.39
1	C	98	THR	N-CA	8.76	1.63	1.46
2	F	388	TYR	CG-CD1	8.75	1.50	1.39
2	F	447	TYR	CB-CG	-8.75	1.38	1.51
1	G	3	GLU	CD-OE2	8.72	1.35	1.25
2	J	450	ARG	CZ-NH1	8.70	1.44	1.33
1	C	165	GLN	CG-CD	8.66	1.71	1.51
2	J	433	SER	CB-OG	8.66	1.53	1.42
2	L	318	LYS	CD-CE	8.62	1.72	1.51
2	D	450	ARG	CZ-NH1	8.61	1.44	1.33
1	I	47	GLU	CG-CD	8.59	1.64	1.51
1	E	120	VAL	CB-CG2	-8.58	1.34	1.52
2	L	479	TYR	CD2-CE2	8.58	1.52	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	168	GLU	CD-OE2	8.54	1.35	1.25
1	G	3	GLU	CD-OE1	8.51	1.35	1.25
1	I	192	GLU	CD-OE1	8.50	1.34	1.25
1	E	168	GLU	CD-OE2	8.49	1.34	1.25
1	I	148	GLU	CD-OE1	8.48	1.34	1.25
1	A	100	ASP	CB-CG	8.48	1.69	1.51
2	J	499	GLU	CD-OE1	8.47	1.34	1.25
1	C	183	TYR	CB-CG	-8.46	1.39	1.51
2	B	473	LYS	CE-NZ	8.45	1.70	1.49
2	H	367	PHE	CE2-CZ	8.44	1.53	1.37
1	E	67	PHE	CE2-CZ	8.44	1.53	1.37
2	L	403	ASN	C-O	8.42	1.39	1.23
1	G	83	TYR	CE1-CZ	8.42	1.49	1.38
1	G	16	TYR	CG-CD1	8.41	1.50	1.39
1	G	154	LYS	CE-NZ	8.41	1.70	1.49
1	G	70	VAL	CB-CG2	-8.41	1.35	1.52
1	A	3	GLU	CD-OE2	8.40	1.34	1.25
2	B	499	GLU	CG-CD	8.39	1.64	1.51
2	D	500	ALA	CA-CB	-8.39	1.34	1.52
1	G	100	ASP	CB-CG	8.38	1.69	1.51
1	E	162	GLU	CD-OE1	8.38	1.34	1.25
2	B	440	ARG	CG-CD	-8.38	1.31	1.51
2	L	345	GLU	CD-OE1	8.38	1.34	1.25
1	G	86	GLU	CD-OE2	8.37	1.34	1.25
1	I	16	TYR	CD2-CE2	8.34	1.51	1.39
2	L	415	TYR	CG-CD2	8.33	1.50	1.39
2	J	390	LYS	CG-CD	8.32	1.80	1.52
1	K	148	GLU	CD-OE1	8.30	1.34	1.25
2	J	414	ARG	NE-CZ	8.29	1.43	1.33
1	C	101	ALA	C-N	8.29	1.48	1.33
1	A	86	GLU	CD-OE2	8.28	1.34	1.25
2	L	380	VAL	CB-CG1	-8.26	1.35	1.52
1	I	99	PHE	CE2-CZ	8.24	1.53	1.37
2	D	449	TRP	CD2-CE2	8.24	1.51	1.41
1	G	103	GLU	CD-OE1	8.23	1.34	1.25
1	K	99	PHE	CD1-CE1	8.21	1.55	1.39
1	A	99	PHE	CD2-CE2	8.20	1.55	1.39
1	K	168	GLU	CD-OE2	8.20	1.34	1.25
1	E	103	GLU	CD-OE1	8.19	1.34	1.25
2	F	338	SER	CB-OG	-8.17	1.31	1.42
2	J	496	ALA	CA-CB	8.17	1.69	1.52
2	L	308	PHE	CD1-CE1	8.17	1.55	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	450	ARG	CZ-NH1	8.17	1.43	1.33
1	K	183	TYR	CD1-CE1	8.16	1.51	1.39
2	D	333	ARG	CZ-NH1	8.15	1.43	1.33
2	H	507	LYS	CD-CE	8.15	1.71	1.51
1	I	162	GLU	CD-OE1	8.15	1.34	1.25
1	C	64	ARG	CZ-NH1	8.11	1.43	1.33
2	J	403	ASN	C-O	8.10	1.38	1.23
1	E	97	THR	CB-CG2	-8.08	1.25	1.52
1	K	79	TYR	CD2-CE2	8.07	1.51	1.39
2	H	304	ASP	CB-CG	8.07	1.68	1.51
1	C	102	GLY	CA-C	8.06	1.64	1.51
2	H	315	TRP	CD2-CE2	8.06	1.51	1.41
2	L	531	ARG	CZ-NH2	8.05	1.43	1.33
2	D	400	TRP	CE3-CZ3	8.04	1.52	1.38
2	J	419	LEU	C-O	8.03	1.38	1.23
2	H	499	GLU	CD-OE1	8.02	1.34	1.25
1	E	86	GLU	CD-OE1	8.02	1.34	1.25
1	I	56	TYR	CG-CD2	8.01	1.49	1.39
1	G	188	ARG	CZ-NH1	8.01	1.43	1.33
2	H	383	ARG	CZ-NH2	8.01	1.43	1.33
1	K	154	LYS	CD-CE	8.00	1.71	1.51
2	H	492	VAL	CB-CG2	-8.00	1.36	1.52
1	I	78	GLU	CD-OE1	8.00	1.34	1.25
1	C	86	GLU	CD-OE2	7.99	1.34	1.25
1	G	180	LYS	CD-CE	7.98	1.71	1.51
1	I	174	ARG	CZ-NH2	7.95	1.43	1.33
1	E	78	GLU	CD-OE2	7.95	1.34	1.25
2	J	368	ASN	N-CA	7.95	1.62	1.46
1	K	69	GLU	CB-CG	-7.95	1.37	1.52
1	C	142	ARG	CG-CD	-7.91	1.32	1.51
2	H	450	ARG	CZ-NH1	7.91	1.43	1.33
2	J	536	GLU	CD-OE1	7.91	1.34	1.25
1	C	16	TYR	CE1-CZ	7.90	1.48	1.38
1	C	192	GLU	CD-OE1	7.89	1.34	1.25
1	E	17	VAL	CB-CG1	7.87	1.69	1.52
1	I	198	PHE	CE2-CZ	7.87	1.52	1.37
2	F	507	LYS	CE-NZ	7.86	1.68	1.49
2	L	436	TYR	CE2-CZ	7.85	1.48	1.38
2	L	536	GLU	CD-OE1	7.85	1.34	1.25
2	D	310	ILE	C-O	7.84	1.38	1.23
2	H	426	VAL	CB-CG2	-7.84	1.36	1.52
1	I	3	GLU	CD-OE2	7.84	1.34	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	83	TYR	CG-CD2	7.84	1.49	1.39
1	C	154	LYS	CE-NZ	7.84	1.68	1.49
1	I	3	GLU	CD-OE1	7.83	1.34	1.25
2	J	450	ARG	CZ-NH2	7.83	1.43	1.33
2	J	499	GLU	CD-OE2	7.83	1.34	1.25
2	L	535	PHE	CE2-CZ	7.82	1.52	1.37
1	A	192	GLU	CD-OE1	7.79	1.34	1.25
2	H	480	PHE	CB-CG	-7.79	1.38	1.51
2	D	390	LYS	CG-CD	7.78	1.78	1.52
1	G	188	ARG	CG-CD	7.77	1.71	1.51
1	E	16	TYR	CE2-CZ	7.76	1.48	1.38
1	C	99	PHE	CB-CG	7.76	1.64	1.51
1	E	155	CYS	CB-SG	7.74	1.95	1.82
1	A	16	TYR	CD1-CE1	7.74	1.50	1.39
1	C	180	LYS	CG-CD	7.73	1.78	1.52
2	F	436	TYR	CD2-CE2	7.73	1.50	1.39
2	H	389	GLY	C-O	-7.72	1.11	1.23
2	D	388	TYR	CD1-CE1	7.71	1.50	1.39
2	D	499	GLU	CD-OE1	7.71	1.34	1.25
1	K	197	PHE	CE2-CZ	7.70	1.51	1.37
2	L	440	ARG	CZ-NH1	7.70	1.43	1.33
1	A	60	GLY	C-O	-7.70	1.11	1.23
2	D	318	LYS	CD-CE	7.69	1.70	1.51
1	E	192	GLU	CD-OE2	7.69	1.34	1.25
1	G	99	PHE	CB-CG	7.69	1.64	1.51
1	E	198	PHE	CE2-CZ	7.68	1.51	1.37
2	J	507	LYS	CE-NZ	7.67	1.68	1.49
1	E	131	PHE	CE2-CZ	7.67	1.51	1.37
2	L	521	TYR	CE1-CZ	7.67	1.48	1.38
1	G	47	GLU	CD-OE1	7.67	1.34	1.25
1	K	183	TYR	CE2-CZ	7.67	1.48	1.38
1	C	99	PHE	CD2-CE2	7.66	1.54	1.39
2	B	439	PHE	CB-CG	-7.65	1.38	1.51
2	D	447	TYR	CD1-CE1	-7.63	1.27	1.39
2	J	481	GLU	CB-CG	-7.63	1.37	1.52
1	C	99	PHE	CD1-CE1	7.63	1.54	1.39
1	G	78	GLU	CD-OE1	7.62	1.34	1.25
1	I	162	GLU	CG-CD	7.61	1.63	1.51
1	A	144	TYR	CE2-CZ	7.61	1.48	1.38
1	G	79	TYR	CG-CD1	7.59	1.49	1.39
1	K	36	TRP	CZ3-CH2	7.59	1.52	1.40
2	L	333	ARG	CZ-NH2	7.59	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	162	GLU	CG-CD	7.59	1.63	1.51
2	B	499	GLU	CD-OE2	7.58	1.33	1.25
1	K	180	LYS	CE-NZ	7.58	1.68	1.49
1	G	78	GLU	CD-OE2	7.57	1.33	1.25
1	G	24	GLU	CG-CD	7.55	1.63	1.51
2	J	409	ARG	CA-C	7.54	1.72	1.52
1	E	163	GLN	CG-CD	7.53	1.68	1.51
1	G	162	GLU	CD-OE1	7.53	1.33	1.25
1	I	175	CYS	CB-SG	7.51	1.95	1.82
2	F	447	TYR	CE1-CZ	7.51	1.48	1.38
2	H	518	CYS	CB-SG	-7.50	1.69	1.82
1	C	185	PHE	CB-CG	-7.48	1.38	1.51
2	B	449	TRP	CG-CD1	7.48	1.47	1.36
1	K	99	PHE	CD2-CE2	7.48	1.54	1.39
1	G	144	TYR	CG-CD1	7.47	1.48	1.39
1	G	180	LYS	CE-NZ	7.47	1.67	1.49
1	C	180	LYS	CE-NZ	7.46	1.67	1.49
2	L	305	ASN	CB-CG	7.45	1.68	1.51
1	G	103	GLU	CG-CD	7.45	1.63	1.51
1	K	44	ALA	CA-CB	7.45	1.68	1.52
1	I	43	ASP	CB-CG	7.44	1.67	1.51
1	K	188	ARG	CZ-NH1	7.44	1.42	1.33
1	E	200	PHE	CG-CD2	7.44	1.50	1.38
2	H	414	ARG	CG-CD	7.43	1.70	1.51
1	C	162	GLU	CG-CD	7.43	1.63	1.51
1	G	38	ARG	CZ-NH1	7.43	1.42	1.33
2	D	324	TYR	CZ-OH	-7.42	1.25	1.37
2	H	318	LYS	CE-NZ	7.42	1.67	1.49
1	E	47	GLU	CD-OE1	7.42	1.33	1.25
1	E	86	GLU	CD-OE2	7.42	1.33	1.25
1	I	168	GLU	CD-OE2	7.42	1.33	1.25
1	A	192	GLU	CD-OE2	7.42	1.33	1.25
1	A	24	GLU	CG-CD	7.39	1.63	1.51
1	A	157	VAL	CB-CG2	-7.38	1.37	1.52
1	G	197	PHE	CD2-CE2	7.38	1.54	1.39
2	L	523	PHE	CD2-CE2	7.38	1.54	1.39
2	F	499	GLU	CD-OE2	7.38	1.33	1.25
1	K	177	VAL	CB-CG2	7.38	1.68	1.52
1	K	183	TYR	CG-CD1	7.38	1.48	1.39
2	J	357	GLY	C-O	7.37	1.35	1.23
1	I	120	VAL	CB-CG2	-7.36	1.37	1.52
1	C	94	ARG	CB-CG	-7.33	1.32	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	390	LYS	CB-CG	-7.31	1.32	1.52
1	E	17	VAL	CB-CG2	7.30	1.68	1.52
2	F	500	ALA	CA-CB	-7.30	1.37	1.52
2	J	368	ASN	CB-CG	7.30	1.67	1.51
1	I	10	SER	CA-CB	7.29	1.63	1.52
1	A	47	GLU	CG-CD	7.28	1.62	1.51
2	F	333	ARG	CZ-NH2	7.28	1.42	1.33
2	F	415	TYR	CG-CD2	7.28	1.48	1.39
2	F	449	TRP	CD2-CE2	7.28	1.50	1.41
2	L	433	SER	CB-OG	7.28	1.51	1.42
1	C	100	ASP	N-CA	7.28	1.60	1.46
2	J	479	TYR	CG-CD1	7.27	1.48	1.39
1	A	103	GLU	CD-OE1	7.27	1.33	1.25
1	E	34	GLU	CD-OE1	7.27	1.33	1.25
1	A	99	PHE	CE1-CZ	7.26	1.51	1.37
1	E	94	ARG	CB-CG	-7.26	1.32	1.52
2	D	305	ASN	CB-CG	7.25	1.67	1.51
1	K	99	PHE	CE1-CZ	7.25	1.51	1.37
1	I	67	PHE	CB-CG	-7.25	1.39	1.51
1	K	86	GLU	CD-OE2	7.24	1.33	1.25
2	D	518	CYS	CB-SG	-7.23	1.70	1.82
2	L	397	VAL	CB-CG2	-7.21	1.37	1.52
2	B	450	ARG	CZ-NH1	7.19	1.42	1.33
1	K	80	GLN	CG-CD	7.19	1.67	1.51
2	D	450	ARG	CZ-NH2	7.18	1.42	1.33
1	A	16	TYR	CD2-CE2	7.18	1.50	1.39
1	E	176	GLU	CD-OE1	7.18	1.33	1.25
2	B	400	TRP	CE3-CZ3	7.17	1.50	1.38
1	G	64	ARG	NE-CZ	7.17	1.42	1.33
2	L	414	ARG	CB-CG	7.17	1.72	1.52
2	D	447	TYR	CE1-CZ	7.16	1.47	1.38
2	J	434	ASP	CG-OD2	7.16	1.41	1.25
1	C	34	GLU	CD-OE2	-7.15	1.17	1.25
1	A	178	ASP	CB-CG	7.15	1.66	1.51
1	K	163	GLN	CD-NE2	7.14	1.50	1.32
2	D	436	TYR	CE1-CZ	7.14	1.47	1.38
1	G	197	PHE	CB-CG	-7.14	1.39	1.51
1	I	199	ASP	C-O	7.14	1.36	1.23
1	G	70	VAL	CB-CG1	-7.14	1.37	1.52
1	E	46	GLY	CA-C	-7.14	1.40	1.51
2	J	333	ARG	CZ-NH2	7.14	1.42	1.33
2	H	532	LYS	CA-CB	7.13	1.69	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	154	LYS	CE-NZ	7.12	1.66	1.49
2	H	449	TRP	CD2-CE2	7.10	1.49	1.41
2	F	390	LYS	CE-NZ	7.09	1.66	1.49
1	C	67	PHE	CB-CG	-7.09	1.39	1.51
1	K	104	TRP	CZ3-CH2	7.08	1.51	1.40
1	K	144	TYR	CD2-CE2	7.08	1.50	1.39
2	L	447	TYR	CB-CG	-7.08	1.41	1.51
2	B	523	PHE	CE2-CZ	7.07	1.50	1.37
1	A	34	GLU	CD-OE2	-7.06	1.17	1.25
2	L	369	ASN	C-O	7.05	1.36	1.23
1	E	99	PHE	CD2-CE2	7.05	1.53	1.39
2	B	439	PHE	CE2-CZ	7.04	1.50	1.37
1	I	16	TYR	CZ-OH	7.04	1.49	1.37
1	C	107	HIS	C-O	-7.03	1.10	1.23
2	J	434	ASP	CG-OD1	7.03	1.41	1.25
2	F	380	VAL	CB-CG1	-7.02	1.38	1.52
1	A	188	ARG	CZ-NH1	7.02	1.42	1.33
1	I	148	GLU	CD-OE2	7.02	1.33	1.25
1	G	36	TRP	CE3-CZ3	7.01	1.50	1.38
1	I	78	GLU	CD-OE2	7.01	1.33	1.25
1	G	165	GLN	CG-CD	7.01	1.67	1.51
2	D	391	PRO	CB-CG	-7.01	1.15	1.50
2	F	306	SER	CB-OG	-7.00	1.33	1.42
2	B	437	TYR	CE2-CZ	-7.00	1.29	1.38
1	K	40	ALA	C-O	7.00	1.36	1.23
2	H	337	VAL	N-CA	6.99	1.60	1.46
1	K	198	PHE	CE2-CZ	6.99	1.50	1.37
2	F	411	LYS	CG-CD	6.98	1.76	1.52
1	E	99	PHE	CG-CD2	6.98	1.49	1.38
2	H	367	PHE	CG-CD1	6.97	1.49	1.38
1	K	89	PHE	C-O	6.96	1.36	1.23
2	J	377	ARG	CZ-NH2	6.96	1.42	1.33
2	B	535	PHE	CD1-CE1	6.96	1.53	1.39
1	E	38	ARG	CG-CD	6.96	1.69	1.51
1	G	133	ARG	CB-CG	-6.96	1.33	1.52
1	I	131	PHE	CE2-CZ	6.95	1.50	1.37
2	J	493	LYS	CE-NZ	6.95	1.66	1.49
2	B	381	ALA	CA-CB	-6.95	1.37	1.52
2	L	481	GLU	CD-OE2	6.95	1.33	1.25
1	K	196	VAL	CB-CG2	-6.94	1.38	1.52
2	D	306	SER	C-O	-6.93	1.10	1.23
1	G	192	GLU	CD-OE1	6.93	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	436	TYR	CZ-OH	6.93	1.49	1.37
1	E	144	TYR	CD2-CE2	6.92	1.49	1.39
2	D	370	GLY	C-O	6.91	1.34	1.23
2	H	499	GLU	CB-CG	-6.91	1.39	1.52
1	E	16	TYR	CE1-CZ	6.91	1.47	1.38
2	D	388	TYR	CZ-OH	6.91	1.49	1.37
2	F	414	ARG	CB-CG	6.91	1.71	1.52
2	L	536	GLU	CG-CD	6.91	1.62	1.51
1	E	200	PHE	CE2-CZ	6.90	1.50	1.37
1	G	163	GLN	CG-CD	6.90	1.67	1.51
2	L	312	ASP	CB-CG	6.90	1.66	1.51
2	F	440	ARG	CZ-NH2	-6.90	1.24	1.33
2	D	366	ASN	C-O	-6.89	1.10	1.23
2	B	311	ARG	CZ-NH1	6.89	1.42	1.33
1	E	177	VAL	CB-CG1	6.89	1.67	1.52
1	C	168	GLU	CD-OE2	6.89	1.33	1.25
1	I	163	GLN	CG-CD	6.88	1.66	1.51
2	B	411	LYS	CD-CE	6.87	1.68	1.51
1	G	144	TYR	C-O	6.87	1.36	1.23
1	G	104	TRP	CE3-CZ3	6.86	1.50	1.38
1	C	154	LYS	CD-CE	6.86	1.68	1.51
1	I	188	ARG	CB-CG	-6.86	1.34	1.52
1	E	148	GLU	CB-CG	-6.86	1.39	1.52
2	L	508	LEU	C-O	-6.85	1.10	1.23
2	B	436	TYR	CD2-CE2	6.85	1.49	1.39
2	D	525	ILE	CA-CB	-6.85	1.39	1.54
1	G	16	TYR	C-O	6.84	1.36	1.23
1	I	3	GLU	CG-CD	6.84	1.62	1.51
1	K	192	GLU	CG-CD	6.84	1.62	1.51
1	I	83	TYR	CG-CD1	-6.83	1.30	1.39
1	A	38	ARG	CZ-NH1	6.83	1.42	1.33
1	C	41	LYS	CE-NZ	6.83	1.66	1.49
2	H	417	ALA	CA-CB	-6.83	1.38	1.52
2	L	531	ARG	CZ-NH1	6.81	1.41	1.33
1	K	144	TYR	CG-CD1	6.80	1.48	1.39
1	E	110	LYS	CD-CE	-6.80	1.34	1.51
1	C	109	VAL	CB-CG2	-6.80	1.38	1.52
1	I	97	THR	C-O	6.80	1.36	1.23
2	L	414	ARG	NE-CZ	6.79	1.41	1.33
2	D	428	ARG	CA-C	-6.79	1.35	1.52
1	E	192	GLU	CD-OE1	6.79	1.33	1.25
1	K	88	ALA	CA-CB	6.78	1.66	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	91	SER	CB-OG	-6.78	1.33	1.42
2	H	461	ILE	CA-CB	-6.77	1.39	1.54
1	G	88	ALA	CA-CB	-6.76	1.38	1.52
1	E	189	ILE	N-CA	-6.75	1.32	1.46
2	B	308	PHE	CE1-CZ	6.74	1.50	1.37
2	D	493	LYS	CE-NZ	6.74	1.66	1.49
2	H	390	LYS	CE-NZ	6.74	1.66	1.49
1	E	198	PHE	CD1-CE1	6.74	1.52	1.39
1	E	96	ALA	CA-CB	-6.73	1.38	1.52
2	F	333	ARG	CZ-NH1	6.73	1.41	1.33
2	L	400	TRP	CG-CD1	6.73	1.46	1.36
1	I	92	PHE	CG-CD2	6.73	1.48	1.38
1	I	86	GLU	CD-OE1	6.73	1.33	1.25
2	L	443	LYS	CE-NZ	6.73	1.65	1.49
2	B	414	ARG	CZ-NH2	6.72	1.41	1.33
1	K	192	GLU	CB-CG	6.72	1.65	1.52
2	L	438	SER	CB-OG	-6.72	1.33	1.42
1	G	132	ALA	CA-CB	-6.72	1.38	1.52
1	I	83	TYR	CG-CD2	6.71	1.47	1.39
2	H	439	PHE	CB-CG	-6.71	1.40	1.51
1	E	47	GLU	CD-OE2	6.71	1.33	1.25
1	E	70	VAL	CB-CG2	-6.71	1.38	1.52
1	G	163	GLN	CD-OE1	6.70	1.38	1.24
1	K	13	ALA	CA-CB	-6.70	1.38	1.52
1	E	131	PHE	CG-CD2	6.70	1.48	1.38
1	G	196	VAL	CB-CG1	-6.70	1.38	1.52
1	C	47	GLU	C-O	-6.68	1.10	1.23
1	G	185	PHE	CD2-CE2	6.68	1.52	1.39
2	H	493	LYS	CE-NZ	6.68	1.65	1.49
2	F	351	PHE	CB-CG	-6.67	1.40	1.51
1	K	177	VAL	CB-CG1	6.67	1.66	1.52
1	A	24	GLU	CD-OE1	6.67	1.32	1.25
1	C	194	GLU	CD-OE1	6.67	1.32	1.25
1	G	65	ASP	CA-CB	-6.67	1.39	1.53
1	G	98	THR	N-CA	6.66	1.59	1.46
1	K	34	GLU	CG-CD	6.65	1.61	1.51
1	E	71	TRP	CE3-CZ3	6.64	1.49	1.38
2	L	301	PRO	CG-CD	6.64	1.72	1.50
1	A	103	GLU	C-O	-6.64	1.10	1.23
2	L	383	ARG	CZ-NH2	6.63	1.41	1.33
2	J	324	TYR	CD2-CE2	6.62	1.49	1.39
2	J	415	TYR	CG-CD2	6.62	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	538	CYS	CA-C	6.61	1.70	1.52
1	E	56	TYR	CE1-CZ	6.60	1.47	1.38
2	L	499	GLU	CD-OE2	6.60	1.32	1.25
1	K	3	GLU	CD-OE1	6.60	1.32	1.25
2	L	315	TRP	CZ3-CH2	6.59	1.50	1.40
2	H	398	GLU	CB-CG	-6.58	1.39	1.52
1	K	99	PHE	CE2-CZ	6.58	1.49	1.37
1	C	34	GLU	CB-CG	-6.58	1.39	1.52
2	H	538	CYS	CB-SG	-6.57	1.71	1.82
1	I	74	ASP	C-O	6.57	1.35	1.23
2	H	523	PHE	CD1-CE1	6.56	1.52	1.39
2	J	411	LYS	CE-NZ	6.56	1.65	1.49
1	C	188	ARG	NE-CZ	6.55	1.41	1.33
2	B	315	TRP	CG-CD1	-6.55	1.27	1.36
2	D	368	ASN	C-O	6.55	1.35	1.23
2	F	430	LEU	C-O	-6.55	1.10	1.23
1	I	144	TYR	CD2-CE2	6.54	1.49	1.39
1	E	100	ASP	CB-CG	6.54	1.65	1.51
2	B	344	SER	CA-CB	-6.54	1.43	1.52
1	K	56	TYR	CD2-CE2	6.54	1.49	1.39
2	F	397	VAL	CB-CG2	-6.54	1.39	1.52
1	C	177	VAL	CB-CG2	-6.53	1.39	1.52
2	J	354	LEU	C-O	6.53	1.35	1.23
2	L	440	ARG	CG-CD	-6.53	1.35	1.51
1	I	189	ILE	CA-CB	-6.52	1.39	1.54
2	L	357	GLY	C-O	6.52	1.34	1.23
1	K	144	TYR	CE1-CZ	6.50	1.47	1.38
1	E	46	GLY	C-O	-6.50	1.13	1.23
2	F	398	GLU	CG-CD	6.50	1.61	1.51
1	K	192	GLU	CD-OE2	6.50	1.32	1.25
1	K	27	GLY	C-O	6.50	1.34	1.23
2	J	318	LYS	C-O	6.49	1.35	1.23
1	E	16	TYR	CB-CG	6.49	1.61	1.51
2	H	354	LEU	C-O	6.49	1.35	1.23
1	E	79	TYR	CE1-CZ	6.49	1.47	1.38
1	A	162	GLU	CD-OE2	6.49	1.32	1.25
1	C	185	PHE	CE2-CZ	6.49	1.49	1.37
1	K	181	THR	C-O	6.48	1.35	1.23
2	B	398	GLU	CB-CG	-6.47	1.39	1.52
1	G	65	ASP	C-O	6.47	1.35	1.23
1	A	56	TYR	CE1-CZ	6.47	1.47	1.38
2	B	509	ASP	C-O	6.47	1.35	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	176	GLU	CD-OE1	6.47	1.32	1.25
2	B	397	VAL	CB-CG2	-6.46	1.39	1.52
2	B	436	TYR	CG-CD1	6.46	1.47	1.39
2	L	501	VAL	CB-CG2	-6.46	1.39	1.52
1	G	7	GLU	CD-OE1	6.46	1.32	1.25
2	J	414	ARG	CZ-NH1	6.46	1.41	1.33
1	K	178	ASP	C-O	6.45	1.35	1.23
2	B	345	GLU	CG-CD	-6.45	1.42	1.51
1	G	197	PHE	CG-CD1	6.45	1.48	1.38
1	A	101	ALA	C-N	6.45	1.44	1.33
2	J	482	GLY	CA-C	6.44	1.62	1.51
2	B	370	GLY	C-O	6.44	1.33	1.23
2	D	499	GLU	CG-CD	6.44	1.61	1.51
2	B	338	SER	CA-CB	-6.44	1.43	1.52
1	I	35	ILE	CB-CG2	-6.44	1.32	1.52
1	K	89	PHE	CE1-CZ	6.44	1.49	1.37
1	K	80	GLN	C-O	6.43	1.35	1.23
2	L	450	ARG	CZ-NH2	6.43	1.41	1.33
2	D	304	ASP	CB-CG	6.43	1.65	1.51
1	K	99	PHE	CG-CD1	6.43	1.48	1.38
2	B	486	ILE	CB-CG2	-6.43	1.32	1.52
1	E	38	ARG	CZ-NH1	6.43	1.41	1.33
1	G	99	PHE	CG-CD2	6.43	1.48	1.38
2	B	414	ARG	CG-CD	6.42	1.68	1.51
1	G	99	PHE	CG-CD1	6.42	1.48	1.38
2	H	450	ARG	CZ-NH2	6.42	1.41	1.33
1	I	165	GLN	CG-CD	6.42	1.65	1.51
1	A	159	ASN	CB-CG	6.42	1.65	1.51
1	G	144	TYR	CD1-CE1	6.42	1.49	1.39
1	K	144	TYR	CD1-CE1	6.42	1.49	1.39
1	I	99	PHE	CD1-CE1	6.42	1.52	1.39
1	E	55	VAL	CB-CG1	-6.42	1.39	1.52
2	L	475	ILE	C-O	6.41	1.35	1.23
2	H	385	VAL	C-O	6.40	1.35	1.23
1	K	17	VAL	CB-CG2	6.40	1.66	1.52
1	A	149	ALA	CA-CB	-6.39	1.39	1.52
2	D	537	ASN	N-CA	6.39	1.59	1.46
1	G	94	ARG	CB-CG	-6.39	1.35	1.52
2	B	369	ASN	C-O	6.39	1.35	1.23
1	E	103	GLU	CG-CD	6.39	1.61	1.51
2	H	403	ASN	C-O	6.39	1.35	1.23
2	L	420	ASP	C-O	6.38	1.35	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	356	PHE	CE1-CZ	6.38	1.49	1.37
2	B	532	LYS	C-O	6.37	1.35	1.23
1	G	101	ALA	CA-CB	6.37	1.65	1.52
1	G	47	GLU	CG-CD	6.37	1.61	1.51
1	C	83	TYR	CG-CD2	6.37	1.47	1.39
2	F	370	GLY	C-O	6.37	1.33	1.23
2	H	499	GLU	CD-OE2	6.36	1.32	1.25
2	J	522	ARG	CZ-NH1	6.36	1.41	1.33
2	H	521	TYR	CE2-CZ	6.36	1.46	1.38
2	B	536	GLU	C-O	6.35	1.35	1.23
1	I	100	ASP	CB-CG	6.35	1.65	1.51
1	A	99	PHE	CD1-CE1	6.34	1.51	1.39
2	J	442	ILE	CB-CG2	6.34	1.72	1.52
2	L	390	LYS	CE-NZ	6.34	1.65	1.49
1	E	99	PHE	CE2-CZ	6.34	1.49	1.37
2	J	415	TYR	CD1-CE1	6.33	1.48	1.39
1	G	176	GLU	CG-CD	6.32	1.61	1.51
2	D	433	SER	CB-OG	6.32	1.50	1.42
2	H	503	GLN	CA-CB	-6.32	1.40	1.53
1	I	41	LYS	CE-NZ	6.32	1.64	1.49
1	K	115	ASN	CG-OD1	6.32	1.37	1.24
1	A	192	GLU	CG-CD	6.32	1.61	1.51
2	F	494	SER	CB-OG	6.32	1.50	1.42
2	B	414	ARG	NE-CZ	6.32	1.41	1.33
1	C	78	GLU	CD-OE1	6.31	1.32	1.25
1	G	114	VAL	CB-CG2	-6.31	1.39	1.52
2	J	376	GLU	CB-CG	-6.30	1.40	1.52
2	D	363	LEU	CG-CD2	-6.30	1.28	1.51
2	J	536	GLU	CD-OE2	6.30	1.32	1.25
1	K	101	ALA	CA-CB	6.30	1.65	1.52
1	A	99	PHE	CG-CD2	6.29	1.48	1.38
2	L	352	SER	C-O	6.29	1.35	1.23
1	K	155	CYS	C-O	6.28	1.35	1.23
1	G	67	PHE	CG-CD1	6.27	1.48	1.38
1	E	188	ARG	CB-CG	-6.27	1.35	1.52
2	L	535	PHE	CE1-CZ	6.27	1.49	1.37
1	K	183	TYR	CD2-CE2	6.26	1.48	1.39
1	E	150	GLN	CD-OE1	6.26	1.37	1.24
1	I	99	PHE	CD2-CE2	6.24	1.51	1.39
2	H	345	GLU	CB-CG	-6.24	1.40	1.52
1	I	56	TYR	CB-CG	-6.23	1.42	1.51
2	D	389	GLY	C-O	-6.23	1.13	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	532	LYS	CA-CB	6.21	1.67	1.53
2	D	538	CYS	CA-C	6.20	1.69	1.52
1	E	142	ARG	CG-CD	-6.20	1.36	1.51
2	B	414	ARG	CB-CG	6.20	1.69	1.52
2	J	482	GLY	C-O	6.20	1.33	1.23
2	B	324	TYR	CG-CD1	6.20	1.47	1.39
2	D	501	VAL	CB-CG2	6.20	1.65	1.52
1	E	66	SER	CB-OG	-6.20	1.34	1.42
2	L	400	TRP	CZ3-CH2	6.19	1.50	1.40
1	C	198	PHE	CG-CD1	6.19	1.48	1.38
2	J	538	CYS	CA-C	6.19	1.69	1.52
1	C	69	GLU	C-O	6.19	1.35	1.23
1	E	167	ARG	CB-CG	-6.19	1.35	1.52
2	D	439	PHE	CE1-CZ	-6.18	1.25	1.37
1	I	98	THR	N-CA	6.18	1.58	1.46
2	F	472	THR	CB-CG2	-6.18	1.31	1.52
1	I	188	ARG	NE-CZ	6.17	1.41	1.33
2	B	376	GLU	CG-CD	6.17	1.61	1.51
2	J	396	LEU	C-O	6.17	1.35	1.23
1	C	99	PHE	CG-CD2	6.17	1.48	1.38
2	L	448	PRO	C-O	6.17	1.35	1.23
1	G	56	TYR	CG-CD1	6.17	1.47	1.39
1	A	150	GLN	CG-CD	6.16	1.65	1.51
2	F	415	TYR	CE2-CZ	6.16	1.46	1.38
2	J	322	PRO	CG-CD	-6.16	1.30	1.50
1	A	103	GLU	CG-CD	6.16	1.61	1.51
2	B	324	TYR	CA-C	6.15	1.69	1.52
2	J	367	PHE	C-O	6.15	1.35	1.23
2	B	447	TYR	CD2-CE2	-6.14	1.30	1.39
1	C	94	ARG	C-O	-6.14	1.11	1.23
2	J	333	ARG	CZ-NH1	6.14	1.41	1.33
2	F	456	TRP	CE3-CZ3	6.13	1.48	1.38
1	A	144	TYR	CD1-CE1	6.13	1.48	1.39
1	I	120	VAL	CA-CB	-6.13	1.41	1.54
2	F	447	TYR	CE2-CZ	6.13	1.46	1.38
2	H	415	TYR	CG-CD2	6.12	1.47	1.39
2	H	390	LYS	CD-CE	6.12	1.66	1.51
2	J	475	ILE	C-O	6.12	1.34	1.23
1	A	198	PHE	C-O	-6.12	1.11	1.23
1	K	16	TYR	CE1-CZ	6.12	1.46	1.38
1	C	88	ALA	CA-C	6.11	1.68	1.52
2	J	356	PHE	CE1-CZ	6.10	1.49	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	34	GLU	CB-CG	-6.10	1.40	1.52
2	J	462	HIS	CA-CB	-6.10	1.40	1.53
2	D	522	ARG	CZ-NH2	6.09	1.41	1.33
2	F	532	LYS	N-CA	6.09	1.58	1.46
2	H	308	PHE	CE1-CZ	6.09	1.49	1.37
2	J	456	TRP	CE3-CZ3	-6.08	1.28	1.38
2	D	479	TYR	CD2-CE2	6.08	1.48	1.39
2	F	376	GLU	CD-OE1	6.08	1.32	1.25
2	J	535	PHE	CE2-CZ	6.08	1.48	1.37
2	D	390	LYS	CA-C	-6.08	1.37	1.52
1	C	24	GLU	CG-CD	6.06	1.61	1.51
2	J	384	VAL	CA-CB	6.06	1.67	1.54
1	E	188	ARG	NE-CZ	6.06	1.41	1.33
2	L	337	VAL	CB-CG1	-6.06	1.40	1.52
2	F	436	TYR	CD1-CE1	6.05	1.48	1.39
1	G	178	ASP	CB-CG	6.05	1.64	1.51
1	K	57	ASP	C-O	6.05	1.34	1.23
1	C	106	LEU	CA-CB	-6.05	1.39	1.53
1	K	71	TRP	C-O	6.05	1.34	1.23
1	C	83	TYR	CD1-CE1	6.04	1.48	1.39
2	D	318	LYS	CG-CD	6.04	1.73	1.52
2	H	415	TYR	CD1-CE1	6.04	1.48	1.39
2	D	434	ASP	C-O	6.03	1.34	1.23
2	B	351	PHE	CG-CD2	6.03	1.47	1.38
1	E	134	GLY	N-CA	-6.03	1.37	1.46
1	E	78	GLU	CD-OE1	6.02	1.32	1.25
2	H	380	VAL	CB-CG2	-6.01	1.40	1.52
1	I	16	TYR	CG-CD1	6.01	1.47	1.39
2	J	449	TRP	CG-CD1	6.01	1.45	1.36
2	L	447	TYR	CE1-CZ	6.01	1.46	1.38
2	F	525	ILE	CA-CB	-6.00	1.41	1.54
1	G	26	ALA	CA-CB	6.00	1.65	1.52
1	G	188	ARG	C-O	6.00	1.34	1.23
1	G	183	TYR	CG-CD2	5.99	1.47	1.39
2	L	532	LYS	C-O	5.99	1.34	1.23
1	I	89	PHE	CE1-CZ	5.99	1.48	1.37
1	K	101	ALA	C-N	5.99	1.43	1.33
1	E	117	ALA	CA-CB	-5.99	1.39	1.52
1	K	188	ARG	CZ-NH2	5.99	1.40	1.33
2	J	308	PHE	CB-CG	-5.98	1.41	1.51
1	C	97	THR	CB-CG2	-5.98	1.32	1.52
2	F	503	GLN	CB-CG	-5.97	1.36	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	64	ARG	C-O	-5.97	1.12	1.23
1	K	154	LYS	CE-NZ	5.97	1.64	1.49
2	F	480	PHE	CB-CG	-5.97	1.41	1.51
2	L	412	ASN	CB-CG	5.97	1.64	1.51
1	G	63	VAL	CB-CG1	-5.96	1.40	1.52
2	J	447	TYR	CB-CG	-5.96	1.42	1.51
1	K	91	SER	CA-CB	-5.96	1.44	1.52
1	A	70	VAL	CB-CG1	-5.95	1.40	1.52
1	K	64	ARG	NE-CZ	5.94	1.40	1.33
1	K	150	GLN	CD-OE1	5.94	1.37	1.24
2	L	351	PHE	CD1-CE1	5.94	1.51	1.39
2	L	414	ARG	CD-NE	5.94	1.56	1.46
2	H	414	ARG	NE-CZ	5.94	1.40	1.33
2	J	481	GLU	CD-OE1	5.94	1.32	1.25
1	K	145	PHE	CB-CG	-5.93	1.41	1.51
2	L	398	GLU	CG-CD	5.93	1.60	1.51
2	F	501	VAL	CB-CG2	-5.93	1.40	1.52
2	H	523	PHE	CB-CG	-5.93	1.41	1.51
2	L	417	ALA	CA-CB	-5.93	1.40	1.52
2	D	457	ARG	CB-CG	-5.92	1.36	1.52
2	L	415	TYR	CD2-CE2	5.92	1.48	1.39
2	D	493	LYS	CD-CE	5.92	1.66	1.51
1	I	24	GLU	CD-OE2	5.92	1.32	1.25
1	A	92	PHE	CG-CD1	5.91	1.47	1.38
1	E	9	PRO	CB-CG	-5.91	1.20	1.50
1	G	56	TYR	CE1-CZ	5.91	1.46	1.38
2	F	416	LEU	CG-CD2	5.90	1.73	1.51
2	L	390	LYS	CD-CE	5.90	1.66	1.51
2	D	334	GLN	CG-CD	5.90	1.64	1.51
1	I	99	PHE	CG-CD1	5.90	1.47	1.38
2	L	516	MET	SD-CE	5.90	2.10	1.77
1	C	79	TYR	CD2-CE2	5.90	1.48	1.39
2	D	318	LYS	CB-CG	5.89	1.68	1.52
2	D	430	LEU	C-O	-5.89	1.12	1.23
1	A	102	GLY	N-CA	5.89	1.54	1.46
1	A	165	GLN	CG-CD	5.89	1.64	1.51
1	E	99	PHE	CB-CG	5.89	1.61	1.51
1	E	162	GLU	CB-CG	-5.89	1.41	1.52
1	G	162	GLU	CG-CD	5.89	1.60	1.51
2	F	450	ARG	CZ-NH2	5.89	1.40	1.33
2	L	535	PHE	CD2-CE2	5.87	1.50	1.39
1	C	198	PHE	CD1-CE1	5.87	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	103	GLU	CD-OE1	5.86	1.32	1.25
2	D	521	TYR	CG-CD2	5.85	1.46	1.39
1	K	119	GLY	CA-C	5.84	1.61	1.51
2	H	522	ARG	CB-CG	-5.83	1.36	1.52
1	I	169	THR	C-O	-5.83	1.12	1.23
2	F	532	LYS	CA-C	5.83	1.68	1.52
2	F	388	TYR	CE2-CZ	5.83	1.46	1.38
2	F	459	ALA	C-O	5.82	1.34	1.23
1	I	191	GLY	C-O	5.82	1.32	1.23
2	L	532	LYS	CA-C	5.82	1.68	1.52
1	C	183	TYR	CD2-CE2	5.82	1.48	1.39
1	K	38	ARG	CG-CD	5.82	1.66	1.51
2	F	522	ARG	CB-CG	-5.82	1.36	1.52
1	C	176	GLU	CG-CD	-5.81	1.43	1.51
2	J	390	LYS	CE-NZ	5.81	1.63	1.49
1	I	142	ARG	CG-CD	-5.81	1.37	1.51
2	J	414	ARG	CD-NE	5.81	1.56	1.46
1	E	166	ARG	CG-CD	-5.80	1.37	1.51
2	J	358	ALA	CA-CB	5.80	1.64	1.52
1	E	150	GLN	CG-CD	5.80	1.64	1.51
2	H	525	ILE	CB-CG2	5.80	1.70	1.52
2	D	380	VAL	CA-CB	5.79	1.67	1.54
1	K	45	PRO	C-O	5.79	1.34	1.23
2	L	423	PHE	C-O	5.79	1.34	1.23
1	I	83	TYR	CD2-CE2	5.79	1.48	1.39
1	E	98	THR	N-CA	5.78	1.57	1.46
1	A	73	ALA	CA-CB	-5.78	1.40	1.52
2	D	351	PHE	CE2-CZ	5.78	1.48	1.37
1	I	7	GLU	CD-OE2	5.78	1.32	1.25
2	L	371	GLY	C-O	5.78	1.32	1.23
1	I	99	PHE	CG-CD2	5.78	1.47	1.38
1	K	184	ARG	CZ-NH2	5.78	1.40	1.33
1	G	7	GLU	C-O	5.77	1.34	1.23
1	E	99	PHE	CG-CD1	5.77	1.47	1.38
1	C	109	VAL	CB-CG1	-5.77	1.40	1.52
2	B	424	GLY	CA-C	5.76	1.61	1.51
2	J	457	ARG	CZ-NH1	5.76	1.40	1.33
2	D	536	GLU	C-O	5.76	1.34	1.23
2	F	399	MET	CA-CB	-5.76	1.41	1.53
2	F	411	LYS	CD-CE	5.75	1.65	1.51
1	E	94	ARG	C-O	-5.75	1.12	1.23
2	J	414	ARG	CG-CD	5.75	1.66	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	439	PHE	CE2-CZ	5.75	1.48	1.37
2	J	502	GLN	CD-NE2	5.75	1.47	1.32
2	J	438	SER	C-O	5.75	1.34	1.23
1	I	72	GLN	CD-NE2	5.74	1.47	1.32
1	K	197	PHE	CB-CG	5.74	1.61	1.51
2	B	411	LYS	CG-CD	5.74	1.72	1.52
2	F	318	LYS	CD-CE	5.74	1.65	1.51
2	H	439	PHE	CD1-CE1	5.73	1.50	1.39
2	H	521	TYR	CE1-CZ	5.73	1.46	1.38
1	C	66	SER	CB-OG	-5.73	1.34	1.42
1	C	180	LYS	CD-CE	5.73	1.65	1.51
1	C	99	PHE	CE1-CZ	5.72	1.48	1.37
1	K	173	LYS	CA-CB	5.72	1.66	1.53
1	C	131	PHE	CD1-CE1	5.72	1.50	1.39
1	I	198	PHE	CB-CG	-5.71	1.41	1.51
2	B	440	ARG	CD-NE	-5.71	1.36	1.46
2	D	417	ALA	CA-CB	-5.70	1.40	1.52
1	K	200	PHE	CG-CD2	5.70	1.47	1.38
1	E	101	ALA	C-N	5.70	1.43	1.33
2	F	368	ASN	CA-CB	5.70	1.68	1.53
1	C	200	PHE	CG-CD1	5.69	1.47	1.38
1	K	143	LEU	C-O	5.69	1.34	1.23
1	K	118	ALA	CA-CB	5.68	1.64	1.52
2	J	376	GLU	CD-OE1	5.68	1.31	1.25
1	I	16	TYR	CE2-CZ	5.68	1.46	1.38
2	F	412	ASN	CB-CG	5.68	1.64	1.51
2	J	499	GLU	CG-CD	5.67	1.60	1.51
1	E	197	PHE	CE1-CZ	5.67	1.48	1.37
2	L	415	TYR	CG-CD1	5.67	1.46	1.39
2	F	414	ARG	NE-CZ	5.67	1.40	1.33
1	K	194	GLU	CD-OE2	5.67	1.31	1.25
1	A	177	VAL	C-O	5.66	1.34	1.23
2	J	411	LYS	CB-CG	5.66	1.67	1.52
1	K	11	GLN	C-O	5.66	1.34	1.23
1	I	83	TYR	CB-CG	5.65	1.60	1.51
1	A	183	TYR	CE1-CZ	5.64	1.45	1.38
1	G	165	GLN	CD-NE2	5.64	1.47	1.32
1	A	26	ALA	CA-CB	5.64	1.64	1.52
1	E	110	LYS	CB-CG	5.63	1.67	1.52
2	J	315	TRP	CE3-CZ3	5.63	1.48	1.38
1	A	91	SER	CB-OG	-5.63	1.34	1.42
1	C	56	TYR	CD1-CE1	-5.63	1.30	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	492	VAL	C-O	-5.63	1.12	1.23
1	A	97	THR	C-O	5.62	1.34	1.23
1	G	149	ALA	CA-CB	-5.62	1.40	1.52
1	C	14	GLY	C-O	5.62	1.32	1.23
2	J	368	ASN	C-O	5.62	1.34	1.23
2	L	334	GLN	CD-OE1	5.62	1.36	1.24
1	K	122	MET	CB-CG	5.62	1.69	1.51
2	F	436	TYR	CE2-CZ	5.62	1.45	1.38
1	I	145	PHE	C-O	5.61	1.34	1.23
2	L	538	CYS	C-OXT	5.61	1.34	1.23
1	E	104	TRP	CZ3-CH2	5.61	1.49	1.40
2	J	351	PHE	CD2-CE2	5.61	1.50	1.39
2	L	328	ILE	CB-CG2	-5.61	1.35	1.52
2	J	388	TYR	CE1-CZ	5.61	1.45	1.38
2	B	434	ASP	N-CA	-5.60	1.35	1.46
1	G	168	GLU	CD-OE2	5.60	1.31	1.25
2	B	328	ILE	C-O	5.60	1.33	1.23
1	G	188	ARG	CZ-NH2	5.60	1.40	1.33
1	A	64	ARG	NE-CZ	5.60	1.40	1.33
1	A	104	TRP	CZ3-CH2	5.60	1.49	1.40
1	A	16	TYR	CE2-CZ	5.60	1.45	1.38
2	D	428	ARG	C-O	-5.59	1.12	1.23
1	C	69	GLU	CD-OE2	-5.59	1.19	1.25
1	C	184	ARG	CZ-NH2	5.59	1.40	1.33
1	E	145	PHE	CB-CG	-5.59	1.41	1.51
2	J	415	TYR	CG-CD1	5.59	1.46	1.39
1	E	137	ILE	C-O	5.59	1.33	1.23
2	H	442	ILE	CB-CG1	-5.59	1.38	1.54
1	G	92	PHE	CG-CD1	5.58	1.47	1.38
1	I	34	GLU	CD-OE1	5.58	1.31	1.25
1	C	22	ALA	CA-CB	5.58	1.64	1.52
1	I	155	CYS	CA-CB	-5.58	1.41	1.53
1	I	36	TRP	CD2-CE2	5.58	1.48	1.41
1	A	32	ASP	CB-CG	5.57	1.63	1.51
1	I	144	TYR	C-O	5.57	1.33	1.23
1	G	38	ARG	NE-CZ	5.56	1.40	1.33
1	K	162	GLU	CD-OE2	5.56	1.31	1.25
2	B	526	VAL	CB-CG1	-5.55	1.41	1.52
1	C	99	PHE	CE2-CZ	5.55	1.47	1.37
2	J	380	VAL	CB-CG2	-5.55	1.41	1.52
2	L	434	ASP	CG-OD1	5.54	1.38	1.25
2	H	440	ARG	CG-CD	-5.54	1.38	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	148	GLU	CG-CD	5.54	1.60	1.51
2	F	489	CYS	CB-SG	-5.53	1.72	1.81
2	H	382	GLY	CA-C	-5.53	1.43	1.51
2	D	441	THR	N-CA	-5.52	1.35	1.46
2	F	388	TYR	CE1-CZ	5.52	1.45	1.38
2	J	509	ASP	CG-OD2	5.52	1.38	1.25
2	H	512	ASN	CG-OD1	5.52	1.36	1.24
1	E	148	GLU	CD-OE1	5.52	1.31	1.25
1	G	34	GLU	CD-OE1	5.52	1.31	1.25
1	C	102	GLY	N-CA	5.52	1.54	1.46
2	D	392	VAL	CA-CB	5.52	1.66	1.54
2	D	480	PHE	CB-CG	-5.52	1.42	1.51
1	G	166	ARG	CB-CG	-5.51	1.37	1.52
1	I	136	ASN	CB-CG	5.50	1.63	1.51
2	B	480	PHE	CB-CG	-5.50	1.42	1.51
1	I	67	PHE	CD2-CE2	5.50	1.50	1.39
1	C	148	GLU	CB-CG	-5.50	1.41	1.52
2	F	336	LEU	C-O	5.50	1.33	1.23
1	K	1	PRO	C-O	5.50	1.34	1.23
2	L	479	TYR	CB-CG	-5.50	1.43	1.51
1	E	142	ARG	CZ-NH1	-5.50	1.25	1.33
2	F	449	TRP	CG-CD1	5.49	1.44	1.36
2	H	351	PHE	CD2-CE2	5.49	1.50	1.39
2	H	470	ILE	CB-CG2	5.49	1.69	1.52
1	G	114	VAL	CA-CB	5.48	1.66	1.54
1	K	177	VAL	CA-CB	5.48	1.66	1.54
2	B	356	PHE	CD2-CE2	5.47	1.50	1.39
1	I	188	ARG	CG-CD	5.47	1.65	1.51
1	E	174	ARG	CA-CB	-5.47	1.42	1.53
2	B	376	GLU	CB-CG	-5.46	1.41	1.52
1	G	142	ARG	CA-CB	-5.46	1.42	1.53
2	D	521	TYR	CE1-CZ	5.46	1.45	1.38
1	I	89	PHE	CG-CD1	5.46	1.47	1.38
1	A	93	GLY	C-O	5.46	1.32	1.23
1	G	189	ILE	C-O	-5.45	1.12	1.23
1	E	80	GLN	CG-CD	5.45	1.63	1.51
1	E	104	TRP	CE3-CZ3	5.45	1.47	1.38
1	C	99	PHE	CG-CD1	5.45	1.47	1.38
1	E	188	ARG	CZ-NH1	5.45	1.40	1.33
1	I	165	GLN	CA-CB	5.44	1.66	1.53
1	K	24	GLU	CD-OE2	5.44	1.31	1.25
1	E	173	LYS	CA-CB	5.44	1.66	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	400	TRP	CE3-CZ3	5.44	1.47	1.38
1	K	129	SER	C-O	5.43	1.33	1.23
1	A	133	ARG	CA-CB	-5.43	1.42	1.53
2	B	337	VAL	C-O	5.43	1.33	1.23
2	F	366	ASN	C-O	-5.43	1.13	1.23
1	C	98	THR	CB-OG1	5.43	1.54	1.43
2	H	473	LYS	CE-NZ	5.43	1.62	1.49
1	E	180	LYS	CD-CE	5.43	1.64	1.51
2	F	456	TRP	CG-CD1	5.42	1.44	1.36
2	J	471	ALA	CA-CB	5.42	1.63	1.52
1	A	3	GLU	CG-CD	5.42	1.60	1.51
2	D	330	ARG	CG-CD	-5.42	1.38	1.51
2	D	351	PHE	CD1-CE1	5.42	1.50	1.39
1	K	176	GLU	CG-CD	5.42	1.60	1.51
2	L	426	VAL	CA-CB	5.41	1.66	1.54
1	I	197	PHE	CE1-CZ	5.41	1.47	1.37
2	B	351	PHE	CE2-CZ	5.41	1.47	1.37
2	B	503	GLN	CA-CB	-5.41	1.42	1.53
2	F	514	ASN	CB-CG	5.41	1.63	1.51
1	K	109	VAL	CA-CB	5.41	1.66	1.54
1	G	64	ARG	CZ-NH1	5.40	1.40	1.33
2	J	415	TYR	CD2-CE2	5.40	1.47	1.39
2	L	414	ARG	CA-CB	5.40	1.65	1.53
2	D	436	TYR	CG-CD1	5.39	1.46	1.39
2	F	423	PHE	CE2-CZ	5.39	1.47	1.37
1	E	150	GLN	CD-NE2	5.39	1.46	1.32
2	D	367	PHE	CG-CD2	5.38	1.46	1.38
1	K	124	PRO	CA-C	5.38	1.63	1.52
2	L	411	LYS	CG-CD	5.38	1.70	1.52
1	K	3	GLU	C-O	5.38	1.33	1.23
2	J	411	LYS	CD-CE	5.38	1.64	1.51
2	F	493	LYS	N-CA	-5.38	1.35	1.46
2	L	315	TRP	CE2-CZ2	5.38	1.48	1.39
1	E	70	VAL	CB-CG1	-5.38	1.41	1.52
1	I	200	PHE	CD2-CE2	5.38	1.50	1.39
2	L	437	TYR	CE1-CZ	5.37	1.45	1.38
1	K	73	ALA	CA-C	5.36	1.66	1.52
1	K	92	PHE	CB-CG	5.36	1.60	1.51
2	L	398	GLU	CD-OE2	-5.36	1.19	1.25
2	F	502	GLN	C-O	-5.36	1.13	1.23
2	F	368	ASN	CB-CG	5.36	1.63	1.51
1	C	183	TYR	CG-CD2	5.35	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	526	VAL	CB-CG2	5.35	1.64	1.52
1	K	92	PHE	CE1-CZ	5.35	1.47	1.37
2	F	522	ARG	CG-CD	-5.35	1.38	1.51
1	K	119	GLY	C-O	5.35	1.32	1.23
1	K	145	PHE	CE1-CZ	5.35	1.47	1.37
2	L	414	ARG	CG-CD	5.35	1.65	1.51
2	H	443	LYS	C-O	-5.35	1.13	1.23
1	K	185	PHE	CG-CD1	5.35	1.46	1.38
2	L	536	GLU	CB-CG	5.34	1.62	1.52
2	B	516	MET	CG-SD	5.34	1.95	1.81
1	C	98	THR	CA-CB	5.34	1.67	1.53
2	H	473	LYS	CG-CD	-5.34	1.34	1.52
2	L	324	TYR	CE2-CZ	5.34	1.45	1.38
2	B	392	VAL	CB-CG2	5.34	1.64	1.52
2	L	319	ALA	CA-CB	-5.34	1.41	1.52
1	A	56	TYR	CZ-OH	5.33	1.47	1.37
1	G	32	ASP	CB-CG	5.33	1.62	1.51
1	G	83	TYR	CD2-CE2	5.33	1.47	1.39
1	A	154	LYS	CD-CE	5.33	1.64	1.51
1	I	129	SER	CA-CB	-5.33	1.45	1.52
2	L	315	TRP	CG-CD1	-5.33	1.29	1.36
2	D	337	VAL	CB-CG2	-5.32	1.41	1.52
1	E	174	ARG	CZ-NH2	5.32	1.40	1.33
1	K	54	GLN	C-O	5.32	1.33	1.23
1	K	33	GLN	CG-CD	5.32	1.63	1.51
1	C	41	LYS	CD-CE	5.32	1.64	1.51
1	C	130	LEU	C-O	5.32	1.33	1.23
2	H	380	VAL	C-O	-5.32	1.13	1.23
1	K	168	GLU	CA-CB	-5.32	1.42	1.53
1	K	70	VAL	CB-CG2	-5.32	1.41	1.52
2	L	528	ARG	CZ-NH1	-5.32	1.26	1.33
2	D	405	GLY	N-CA	-5.31	1.38	1.46
2	D	318	LYS	CE-NZ	5.31	1.62	1.49
2	D	461	ILE	CA-CB	-5.31	1.42	1.54
1	K	36	TRP	CD2-CE2	5.31	1.47	1.41
1	E	22	ALA	CA-CB	5.31	1.63	1.52
1	E	26	ALA	C-O	5.31	1.33	1.23
1	K	97	THR	C-O	5.30	1.33	1.23
1	C	195	THR	N-CA	-5.30	1.35	1.46
1	G	153	ALA	CA-CB	-5.30	1.41	1.52
2	L	414	ARG	CZ-NH1	5.30	1.40	1.33
1	A	24	GLU	CD-OE2	5.30	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	3	GLU	CD-OE1	5.30	1.31	1.25
1	G	55	VAL	CA-CB	-5.30	1.43	1.54
2	J	462	HIS	N-CA	5.30	1.56	1.46
1	A	192	GLU	CB-CG	5.29	1.62	1.52
1	C	56	TYR	C-O	-5.29	1.13	1.23
1	E	75	ALA	CA-CB	-5.29	1.41	1.52
1	K	82	ALA	CA-CB	5.29	1.63	1.52
2	F	400	TRP	CZ3-CH2	5.29	1.48	1.40
1	A	183	TYR	CZ-OH	5.29	1.46	1.37
2	B	333	ARG	CZ-NH1	5.29	1.40	1.33
1	I	180	LYS	CE-NZ	5.29	1.62	1.49
1	C	36	TRP	CG-CD2	5.29	1.52	1.43
1	C	188	ARG	CZ-NH2	5.29	1.40	1.33
2	H	537	ASN	CB-CG	5.29	1.63	1.51
1	K	89	PHE	CB-CG	-5.29	1.42	1.51
1	C	35	ILE	CA-CB	-5.28	1.42	1.54
1	C	63	VAL	CB-CG1	-5.28	1.41	1.52
2	L	484	PRO	CG-CD	5.28	1.68	1.50
2	B	303	GLN	C-O	5.28	1.33	1.23
2	H	377	ARG	CG-CD	-5.28	1.38	1.51
1	E	38	ARG	NE-CZ	5.28	1.40	1.33
1	I	99	PHE	CE1-CZ	5.28	1.47	1.37
2	L	525	ILE	CA-CB	-5.28	1.42	1.54
2	F	415	TYR	CD1-CE1	5.28	1.47	1.39
1	I	71	TRP	CE3-CZ3	5.27	1.47	1.38
1	A	111	PRO	C-O	-5.27	1.12	1.23
1	A	144	TYR	CD2-CE2	5.27	1.47	1.39
2	D	426	VAL	CB-CG1	5.27	1.64	1.52
2	F	378	ILE	N-CA	-5.26	1.35	1.46
2	B	473	LYS	CG-CD	-5.26	1.34	1.52
1	E	185	PHE	CD1-CE1	5.26	1.49	1.39
1	A	91	SER	CA-CB	-5.25	1.45	1.52
1	I	101	ALA	C-N	5.25	1.42	1.33
2	B	394	ASN	CG-ND2	5.25	1.46	1.32
2	H	502	GLN	CD-OE1	5.25	1.35	1.24
2	F	493	LYS	CA-CB	-5.25	1.42	1.53
2	H	459	ALA	CA-CB	-5.25	1.41	1.52
1	C	167	ARG	CA-CB	-5.25	1.42	1.53
2	J	479	TYR	CD2-CE2	5.24	1.47	1.39
2	H	536	GLU	CG-CD	5.24	1.59	1.51
1	A	13	ALA	CA-CB	-5.24	1.41	1.52
1	I	183	TYR	CD2-CE2	5.23	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	16	TYR	CG-CD2	5.23	1.46	1.39
1	A	9	PRO	CG-CD	-5.23	1.33	1.50
2	B	481	GLU	CB-CG	-5.23	1.42	1.52
1	C	100	ASP	CA-CB	5.23	1.65	1.53
2	F	440	ARG	CG-CD	-5.23	1.38	1.51
1	G	190	GLN	N-CA	-5.23	1.35	1.46
1	I	83	TYR	CE1-CZ	5.23	1.45	1.38
1	I	150	GLN	CG-CD	5.23	1.63	1.51
1	K	45	PRO	CA-C	5.23	1.63	1.52
2	D	318	LYS	C-O	5.23	1.33	1.23
2	D	476	THR	N-CA	-5.23	1.35	1.46
1	E	183	TYR	CG-CD2	5.23	1.46	1.39
1	K	197	PHE	CG-CD2	5.23	1.46	1.38
2	D	387	GLN	CB-CG	-5.22	1.38	1.52
1	G	162	GLU	CA-CB	-5.22	1.42	1.53
1	E	197	PHE	CB-CG	-5.22	1.42	1.51
2	F	308	PHE	CD2-CE2	-5.22	1.28	1.39
1	I	176	GLU	CD-OE2	5.21	1.31	1.25
2	H	378	ILE	C-O	-5.21	1.13	1.23
2	B	315	TRP	CE3-CZ3	5.21	1.47	1.38
2	F	382	GLY	CA-C	-5.21	1.43	1.51
1	K	163	GLN	CD-OE1	5.21	1.35	1.24
2	D	367	PHE	CE1-CZ	5.21	1.47	1.37
1	K	171	ILE	N-CA	5.21	1.56	1.46
2	L	499	GLU	CG-CD	5.21	1.59	1.51
1	K	26	ALA	CA-CB	5.20	1.63	1.52
1	A	145	PHE	CG-CD1	5.20	1.46	1.38
1	C	145	PHE	CG-CD2	5.20	1.46	1.38
2	D	403	ASN	C-O	5.20	1.33	1.23
1	A	168	GLU	CA-CB	-5.20	1.42	1.53
2	F	369	ASN	CB-CG	-5.20	1.39	1.51
2	D	486	ILE	CA-CB	-5.20	1.43	1.54
2	B	520	ALA	CA-CB	-5.19	1.41	1.52
2	F	339	ILE	CA-CB	5.19	1.66	1.54
2	D	368	ASN	CB-CG	5.19	1.62	1.51
1	A	185	PHE	C-O	-5.19	1.13	1.23
1	C	65	ASP	CA-CB	-5.18	1.42	1.53
1	E	64	ARG	CZ-NH1	5.18	1.39	1.33
2	F	367	PHE	CE1-CZ	5.18	1.47	1.37
2	H	315	TRP	CB-CG	-5.18	1.41	1.50
2	B	398	GLU	CD-OE2	-5.17	1.20	1.25
1	C	60	GLY	N-CA	-5.17	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	318	LYS	CG-CD	5.17	1.70	1.52
1	G	104	TRP	CZ3-CH2	5.17	1.48	1.40
2	B	502	GLN	CD-NE2	5.17	1.45	1.32
1	G	198	PHE	CG-CD1	5.17	1.46	1.38
2	F	473	LYS	C-O	5.17	1.33	1.23
1	G	17	VAL	C-O	5.17	1.33	1.23
2	J	449	TRP	CD2-CE2	5.17	1.47	1.41
2	J	507	LYS	CG-CD	5.17	1.70	1.52
2	H	439	PHE	CE2-CZ	5.17	1.47	1.37
2	H	414	ARG	CZ-NH1	5.17	1.39	1.33
2	B	492	VAL	C-O	-5.16	1.13	1.23
2	F	315	TRP	CZ3-CH2	5.16	1.48	1.40
2	J	411	LYS	CG-CD	5.16	1.70	1.52
1	A	168	GLU	N-CA	-5.16	1.36	1.46
1	G	100	ASP	CA-CB	5.16	1.65	1.53
1	A	136	ASN	CA-C	-5.15	1.39	1.52
1	K	76	ASN	C-O	5.15	1.33	1.23
1	E	32	ASP	CB-CG	5.15	1.62	1.51
2	J	423	PHE	CG-CD1	5.15	1.46	1.38
1	A	35	ILE	CB-CG2	-5.14	1.36	1.52
2	B	479	TYR	CD2-CE2	5.14	1.47	1.39
2	L	324	TYR	CD2-CE2	5.14	1.47	1.39
2	B	436	TYR	CB-CG	-5.14	1.44	1.51
1	C	144	TYR	CE1-CZ	5.14	1.45	1.38
2	H	456	TRP	CE2-CZ2	-5.14	1.31	1.39
1	G	162	GLU	CB-CG	-5.14	1.42	1.52
1	I	146	ASP	CG-OD2	5.14	1.37	1.25
1	K	128	ILE	C-O	5.14	1.33	1.23
2	B	317	PRO	CA-C	5.14	1.63	1.52
2	J	404	ALA	C-O	5.14	1.33	1.23
2	L	368	ASN	C-O	5.14	1.33	1.23
2	L	450	ARG	CZ-NH1	5.14	1.39	1.33
1	C	114	VAL	CB-CG1	-5.13	1.42	1.52
2	F	329	ALA	CA-CB	5.13	1.63	1.52
1	G	38	ARG	CG-CD	5.13	1.64	1.51
2	L	357	GLY	CA-C	5.13	1.60	1.51
2	L	437	TYR	CD1-CE1	5.13	1.47	1.39
1	A	172	ALA	CA-CB	-5.13	1.41	1.52
2	B	415	TYR	CZ-OH	5.13	1.46	1.37
2	F	441	THR	N-CA	-5.12	1.36	1.46
1	C	163	GLN	CG-CD	5.12	1.62	1.51
1	K	176	GLU	CD-OE2	5.12	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	368	ASN	C-O	5.11	1.33	1.23
2	L	453	PRO	C-O	-5.11	1.13	1.23
1	E	177	VAL	CB-CG2	5.11	1.63	1.52
2	F	400	TRP	CE3-CZ3	5.11	1.47	1.38
1	A	71	TRP	CG-CD1	-5.11	1.29	1.36
2	F	377	ARG	CB-CG	5.11	1.66	1.52
2	J	384	VAL	CB-CG1	-5.10	1.42	1.52
2	J	311	ARG	CZ-NH1	5.10	1.39	1.33
2	J	426	VAL	N-CA	5.10	1.56	1.46
2	F	383	ARG	CB-CG	-5.10	1.38	1.52
2	D	502	GLN	CD-NE2	5.09	1.45	1.32
2	J	521	TYR	CD1-CE1	5.09	1.47	1.39
2	H	318	LYS	CD-CE	5.09	1.64	1.51
2	B	337	VAL	CB-CG2	-5.09	1.42	1.52
1	I	188	ARG	CZ-NH1	5.09	1.39	1.33
1	E	67	PHE	CB-CG	-5.09	1.42	1.51
2	B	434	ASP	CG-OD2	5.08	1.37	1.25
1	G	188	ARG	NE-CZ	5.08	1.39	1.33
2	H	383	ARG	CB-CG	-5.08	1.38	1.52
2	H	305	ASN	CG-OD1	5.08	1.35	1.24
1	I	116	ASN	CB-CG	5.08	1.62	1.51
1	I	174	ARG	CZ-NH1	5.08	1.39	1.33
2	L	350	ASN	N-CA	-5.08	1.36	1.46
1	C	35	ILE	CB-CG2	-5.08	1.37	1.52
2	H	385	VAL	CB-CG2	-5.08	1.42	1.52
2	H	434	ASP	CG-OD1	5.08	1.37	1.25
2	F	305	ASN	CB-CG	5.07	1.62	1.51
1	K	31	ARG	C-O	5.07	1.32	1.23
1	K	1	PRO	CG-CD	5.07	1.67	1.50
1	E	167	ARG	CD-NE	5.06	1.55	1.46
2	J	399	MET	CA-CB	-5.06	1.42	1.53
2	B	483	ASP	C-O	5.06	1.32	1.23
1	C	98	THR	CA-C	5.06	1.66	1.52
2	D	523	PHE	CG-CD1	5.06	1.46	1.38
1	A	142	ARG	CA-CB	-5.06	1.42	1.53
2	F	479	TYR	CE1-CZ	-5.06	1.31	1.38
2	J	456	TRP	CD1-NE1	5.06	1.46	1.38
2	B	449	TRP	CD2-CE2	5.06	1.47	1.41
1	K	131	PHE	CD1-CE1	5.06	1.49	1.39
1	I	116	ASN	CA-C	5.06	1.66	1.52
2	J	342	SER	CB-OG	5.06	1.48	1.42
2	D	414	ARG	NE-CZ	5.05	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	47	GLU	N-CA	-5.05	1.36	1.46
1	K	43	ASP	C-O	5.05	1.32	1.23
2	H	449	TRP	CE2-CZ2	5.05	1.48	1.39
1	K	133	ARG	CB-CG	-5.05	1.39	1.52
2	L	486	ILE	CB-CG2	-5.05	1.37	1.52
2	L	502	GLN	C-O	-5.05	1.13	1.23
2	B	305	ASN	CB-CG	5.04	1.62	1.51
2	D	416	LEU	C-O	5.04	1.32	1.23
2	J	479	TYR	C-O	5.04	1.32	1.23
2	L	535	PHE	CD1-CE1	5.04	1.49	1.39
1	K	16	TYR	CG-CD1	5.04	1.45	1.39
2	F	535	PHE	CG-CD2	5.04	1.46	1.38
2	F	415	TYR	CG-CD1	5.03	1.45	1.39
2	J	361	HIS	C-O	-5.03	1.13	1.23
2	L	537	ASN	CG-OD1	5.03	1.35	1.24
2	D	522	ARG	NE-CZ	5.03	1.39	1.33
2	F	385	VAL	CB-CG2	-5.03	1.42	1.52
1	A	67	PHE	CE2-CZ	5.03	1.47	1.37
2	H	424	GLY	CA-C	5.03	1.59	1.51
2	D	368	ASN	N-CA	5.02	1.56	1.46
1	E	176	GLU	CG-CD	5.02	1.59	1.51
2	F	325	LYS	CE-NZ	-5.02	1.36	1.49
1	K	170	LEU	CG-CD2	5.02	1.70	1.51
2	D	385	VAL	CB-CG2	-5.02	1.42	1.52
1	E	183	TYR	CE1-CZ	5.02	1.45	1.38
1	I	19	ILE	N-CA	-5.02	1.36	1.46
2	D	435	GLY	C-O	-5.01	1.15	1.23
2	F	414	ARG	CG-CD	5.01	1.64	1.51
1	K	7	GLU	CB-CG	5.01	1.61	1.52
1	A	97	THR	CB-CG2	-5.01	1.35	1.52
2	D	484	PRO	CG-CD	-5.01	1.34	1.50
2	B	502	GLN	CD-OE1	5.01	1.34	1.24
2	F	324	TYR	CG-CD1	5.01	1.45	1.39
1	K	92	PHE	C-O	5.01	1.32	1.23
2	J	305	ASN	CB-CG	5.00	1.62	1.51
1	K	120	VAL	CB-CG2	-5.00	1.42	1.52
2	J	414	ARG	CZ-NH2	5.00	1.39	1.33

All (592) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	333	ARG	NE-CZ-NH1	-23.73	108.43	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	133	ARG	NE-CZ-NH1	23.63	132.11	120.30
1	C	94	ARG	NE-CZ-NH1	21.29	130.95	120.30
2	F	440	ARG	NE-CZ-NH2	-20.66	109.97	120.30
2	F	333	ARG	NE-CZ-NH1	-20.45	110.08	120.30
1	I	94	ARG	NE-CZ-NH2	-20.23	110.18	120.30
1	K	64	ARG	NE-CZ-NH1	20.11	130.35	120.30
1	A	94	ARG	NE-CZ-NH1	19.61	130.10	120.30
1	I	133	ARG	NE-CZ-NH2	-19.00	110.80	120.30
2	J	428	ARG	NE-CZ-NH1	18.87	129.73	120.30
1	I	64	ARG	NE-CZ-NH1	18.78	129.69	120.30
2	B	440	ARG	NE-CZ-NH2	-18.65	110.97	120.30
2	J	428	ARG	NE-CZ-NH2	-18.03	111.28	120.30
1	A	94	ARG	NE-CZ-NH2	-17.69	111.45	120.30
2	H	440	ARG	NE-CZ-NH2	-17.35	111.62	120.30
1	K	94	ARG	NE-CZ-NH2	-17.34	111.63	120.30
1	G	94	ARG	NE-CZ-NH2	-16.82	111.89	120.30
1	E	38	ARG	NE-CZ-NH1	16.81	128.70	120.30
1	C	94	ARG	NE-CZ-NH2	-16.54	112.03	120.30
1	K	94	ARG	NE-CZ-NH1	16.39	128.50	120.30
2	F	407	ARG	NE-CZ-NH2	-16.35	112.12	120.30
1	I	64	ARG	NE-CZ-NH2	-15.93	112.34	120.30
1	C	188	ARG	NE-CZ-NH1	15.83	128.21	120.30
2	F	440	ARG	NE-CZ-NH1	15.76	128.18	120.30
1	A	64	ARG	NE-CZ-NH1	15.71	128.15	120.30
1	G	94	ARG	NE-CZ-NH1	15.52	128.06	120.30
1	C	64	ARG	NE-CZ-NH1	15.39	127.99	120.30
1	C	133	ARG	NE-CZ-NH2	-15.32	112.64	120.30
1	K	64	ARG	NE-CZ-NH2	-15.27	112.67	120.30
2	D	428	ARG	NE-CZ-NH2	-15.24	112.68	120.30
2	B	312	ASP	CB-CG-OD1	15.23	132.01	118.30
2	D	440	ARG	NE-CZ-NH1	14.52	127.56	120.30
1	I	94	ARG	NE-CZ-NH1	14.47	127.54	120.30
2	H	440	ARG	NE-CZ-NH1	14.37	127.48	120.30
2	D	440	ARG	NE-CZ-NH2	-14.34	113.13	120.30
1	E	106	LEU	CB-CG-CD2	-14.12	87.00	111.00
2	L	440	ARG	NE-CZ-NH1	14.08	127.34	120.30
1	C	166	ARG	NE-CZ-NH2	-14.04	113.28	120.30
2	H	522	ARG	NE-CZ-NH1	-14.03	113.28	120.30
2	B	428	ARG	NE-CZ-NH2	-13.85	113.37	120.30
2	L	440	ARG	NE-CZ-NH2	-13.74	113.43	120.30
2	D	307	ARG	NE-CZ-NH2	-13.64	113.48	120.30
1	G	38	ARG	NE-CZ-NH1	13.43	127.02	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	457	ARG	NE-CZ-NH2	-13.10	113.75	120.30
2	J	414	ARG	NE-CZ-NH1	13.09	126.85	120.30
2	B	313	ARG	NE-CZ-NH1	12.99	126.80	120.30
1	G	64	ARG	NE-CZ-NH1	12.94	126.77	120.30
2	H	414	ARG	NE-CZ-NH1	12.86	126.73	120.30
2	L	522	ARG	NE-CZ-NH1	-12.70	113.95	120.30
2	B	428	ARG	NE-CZ-NH1	12.58	126.59	120.30
2	B	311	ARG	NE-CZ-NH2	-12.57	114.01	120.30
2	L	528	ARG	NE-CZ-NH1	-12.53	114.04	120.30
1	A	133	ARG	NE-CZ-NH2	-12.46	114.07	120.30
2	J	450	ARG	NE-CZ-NH1	-12.34	114.13	120.30
2	H	538	CYS	CA-CB-SG	-12.23	91.98	114.00
2	L	428	ARG	NE-CZ-NH2	-12.20	114.20	120.30
2	L	428	ARG	NE-CZ-NH1	12.14	126.37	120.30
1	E	188	ARG	NE-CZ-NH1	12.11	126.36	120.30
2	B	434	ASP	CB-CG-OD1	-11.91	107.58	118.30
2	F	333	ARG	NE-CZ-NH2	11.69	126.15	120.30
2	F	312	ASP	CB-CG-OD2	-11.58	107.87	118.30
2	B	430	LEU	CB-CG-CD2	-11.42	91.59	111.00
2	L	414	ARG	NE-CZ-NH1	11.38	125.99	120.30
2	L	407	ARG	NE-CZ-NH1	11.36	125.98	120.30
1	K	133	ARG	NE-CZ-NH1	11.29	125.94	120.30
2	H	528	ARG	NE-CZ-NH1	-11.24	114.68	120.30
2	H	457	ARG	NE-CZ-NH2	-11.17	114.71	120.30
1	G	133	ARG	NE-CZ-NH1	11.16	125.88	120.30
1	A	188	ARG	NE-CZ-NH1	11.15	125.88	120.30
2	F	409	ARG	NE-CZ-NH1	-11.14	114.73	120.30
2	F	407	ARG	NE-CZ-NH1	11.07	125.84	120.30
1	C	166	ARG	NE-CZ-NH1	11.06	125.83	120.30
2	B	473	LYS	CD-CE-NZ	-11.03	86.33	111.70
2	D	473	LYS	CD-CE-NZ	-11.01	86.37	111.70
2	H	450	ARG	NE-CZ-NH1	-10.94	114.83	120.30
2	L	509	ASP	CB-CG-OD2	-10.91	108.48	118.30
2	H	440	ARG	CB-CG-CD	-10.89	83.30	111.60
2	J	377	ARG	NE-CZ-NH1	-10.80	114.90	120.30
1	C	188	ARG	NE-CZ-NH2	-10.80	114.90	120.30
2	D	312	ASP	CB-CG-OD2	-10.78	108.59	118.30
1	C	74	ASP	CB-CG-OD2	-10.74	108.64	118.30
2	F	420	ASP	CB-CG-OD2	-10.70	108.67	118.30
2	F	509	ASP	CB-CG-OD1	10.55	127.79	118.30
1	K	188	ARG	NE-CZ-NH2	-10.50	115.05	120.30
2	B	307	ARG	NE-CZ-NH2	-10.43	115.08	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	142	ARG	NE-CZ-NH2	-10.39	115.11	120.30
2	F	311	ARG	NE-CZ-NH2	-10.28	115.16	120.30
2	D	450	ARG	NE-CZ-NH2	-10.28	115.16	120.30
2	D	428	ARG	NE-CZ-NH1	10.27	125.44	120.30
2	L	333	ARG	NE-CZ-NH2	-10.27	115.16	120.30
1	K	47	GLU	OE1-CD-OE2	10.21	135.56	123.30
1	E	38	ARG	NE-CZ-NH2	-10.16	115.22	120.30
1	C	106	LEU	CB-CG-CD2	-10.15	93.74	111.00
1	I	147	ASP	CB-CG-OD2	-10.15	109.17	118.30
2	F	413	ASP	CB-CG-OD2	10.00	127.30	118.30
2	H	330	ARG	NE-CZ-NH2	-9.99	115.31	120.30
1	I	74	ASP	CB-CG-OD2	-9.94	109.35	118.30
1	E	64	ARG	NE-CZ-NH1	9.92	125.26	120.30
2	F	323	ASP	CB-CG-OD2	-9.92	109.38	118.30
1	G	188	ARG	NE-CZ-NH2	-9.82	115.39	120.30
2	B	538	CYS	CA-CB-SG	-9.81	96.33	114.00
1	A	64	ARG	NE-CZ-NH2	-9.79	115.41	120.30
2	J	434	ASP	CB-CG-OD1	-9.77	109.51	118.30
1	E	57	ASP	CB-CG-OD2	-9.72	109.55	118.30
2	F	455	ASP	CB-CG-OD1	9.71	127.04	118.30
2	F	414	ARG	NE-CZ-NH1	9.69	125.14	120.30
1	G	133	ARG	NE-CZ-NH2	-9.66	115.47	120.30
1	E	166	ARG	NE-CZ-NH2	-9.65	115.48	120.30
1	C	178	ASP	CB-CG-OD1	9.64	126.98	118.30
2	F	507	LYS	CD-CE-NZ	9.60	133.77	111.70
2	H	377	ARG	NE-CZ-NH1	-9.57	115.51	120.30
2	B	312	ASP	CB-CG-OD2	-9.54	109.71	118.30
1	I	147	ASP	CB-CG-OD1	9.51	126.86	118.30
1	I	133	ARG	NE-CZ-NH1	9.49	125.04	120.30
2	H	507	LYS	CD-CE-NZ	9.48	133.50	111.70
1	G	180	LYS	CD-CE-NZ	9.47	133.49	111.70
1	I	167	ARG	NE-CZ-NH2	-9.39	115.60	120.30
2	F	440	ARG	CB-CG-CD	-9.32	87.37	111.60
2	H	311	ARG	NE-CZ-NH2	-9.32	115.64	120.30
2	J	377	ARG	NE-CZ-NH2	9.27	124.93	120.30
2	D	483	ASP	CB-CG-OD1	9.21	126.58	118.30
2	J	447	TYR	CB-CG-CD2	-9.18	115.49	121.00
1	E	65	ASP	CB-CG-OD1	9.15	126.53	118.30
1	A	74	ASP	CB-CG-OD2	9.11	126.50	118.30
1	E	57	ASP	CB-CG-OD1	9.09	126.48	118.30
2	H	473	LYS	CD-CE-NZ	-9.08	90.81	111.70
2	L	473	LYS	CD-CE-NZ	-9.08	90.82	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	186	ASP	CB-CG-OD1	9.05	126.45	118.30
1	E	186	ASP	CB-CG-OD2	-8.98	110.22	118.30
1	G	114	VAL	CG1-CB-CG2	-8.96	96.56	110.90
2	H	311	ARG	NE-CZ-NH1	8.90	124.75	120.30
1	C	184	ARG	NE-CZ-NH2	-8.83	115.89	120.30
2	L	430	LEU	CB-CG-CD2	-8.80	96.05	111.00
2	D	440	ARG	CB-CG-CD	-8.77	88.79	111.60
1	C	64	ARG	NE-CZ-NH2	-8.77	115.92	120.30
1	C	52	LEU	CA-CB-CG	8.76	135.46	115.30
2	F	455	ASP	CB-CG-OD2	-8.76	110.41	118.30
2	L	538	CYS	CA-CB-SG	-8.74	98.26	114.00
2	D	307	ARG	NE-CZ-NH1	8.74	124.67	120.30
2	D	333	ARG	NE-CZ-NH2	8.66	124.63	120.30
1	K	106	LEU	CB-CG-CD1	8.65	125.71	111.00
2	B	377	ARG	NE-CZ-NH1	-8.60	116.00	120.30
1	I	78	GLU	OE1-CD-OE2	8.60	133.62	123.30
2	B	330	ARG	NE-CZ-NH2	-8.55	116.02	120.30
1	C	186	ASP	CB-CG-OD1	8.54	125.98	118.30
2	F	330	ARG	NE-CZ-NH1	8.50	124.55	120.30
2	B	493	LYS	CD-CE-NZ	8.47	131.19	111.70
2	H	383	ARG	NE-CZ-NH1	-8.46	116.07	120.30
1	A	188	ARG	NE-CZ-NH2	-8.45	116.08	120.30
2	H	312	ASP	CB-CG-OD2	-8.44	110.70	118.30
1	E	166	ARG	NE-CZ-NH1	8.40	124.50	120.30
1	A	52	LEU	CA-CB-CG	8.39	134.59	115.30
2	D	426	VAL	CB-CA-C	-8.36	95.52	111.40
2	B	457	ARG	NE-CZ-NH1	8.31	124.46	120.30
2	D	524	ASP	CB-CG-OD1	8.27	125.75	118.30
2	F	457	ARG	NE-CZ-NH2	-8.25	116.17	120.30
2	J	365	LEU	CB-CG-CD1	-8.25	96.98	111.00
2	L	328	ILE	CG1-CB-CG2	-8.22	93.32	111.40
2	D	493	LYS	CD-CE-NZ	8.20	130.57	111.70
2	H	434	ASP	CB-CG-OD1	-8.19	110.93	118.30
1	A	180	LYS	CD-CE-NZ	8.15	130.46	111.70
2	D	330	ARG	NE-CZ-NH2	-8.15	116.23	120.30
2	H	312	ASP	CB-CG-OD1	8.11	125.60	118.30
2	F	485	LEU	CB-CG-CD1	8.09	124.76	111.00
1	A	133	ARG	NE-CZ-NH1	8.08	124.34	120.30
1	G	65	ASP	CB-CG-OD1	8.08	125.57	118.30
1	G	188	ARG	NE-CZ-NH1	8.05	124.32	120.30
2	B	528	ARG	NE-CZ-NH1	-8.03	116.28	120.30
1	C	167	ARG	NE-CZ-NH1	-8.02	116.29	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	323	ASP	CB-CG-OD1	7.99	125.50	118.30
2	L	455	ASP	CB-CG-OD2	-7.96	111.13	118.30
2	H	328	ILE	CG1-CB-CG2	-7.95	93.92	111.40
2	D	386	ASP	CB-CG-OD1	-7.93	111.17	118.30
1	E	64	ARG	NE-CZ-NH2	-7.93	116.34	120.30
1	K	160	LEU	CB-CG-CD1	-7.92	97.53	111.00
1	C	114	VAL	CG1-CB-CG2	-7.90	98.26	110.90
1	I	167	ARG	NE-CZ-NH1	7.89	124.25	120.30
2	J	311	ARG	CG-CD-NE	-7.87	95.27	111.80
2	J	416	LEU	CB-CG-CD1	-7.83	97.70	111.00
1	G	38	ARG	NE-CZ-NH2	-7.82	116.39	120.30
1	E	81	ASP	CB-CG-OD2	-7.80	111.28	118.30
1	K	100	ASP	CB-CG-OD2	-7.80	111.28	118.30
2	L	509	ASP	CB-CG-OD1	7.80	125.32	118.30
1	E	69	GLU	OE1-CD-OE2	-7.78	113.96	123.30
2	F	473	LYS	CD-CE-NZ	-7.77	93.82	111.70
2	L	475	ILE	CG1-CB-CG2	-7.77	94.30	111.40
2	F	428	ARG	NE-CZ-NH1	7.77	124.19	120.30
2	H	457	ARG	NE-CZ-NH1	7.74	124.17	120.30
2	L	343	ILE	CG1-CB-CG2	-7.73	94.39	111.40
1	G	23	LEU	CB-CG-CD2	-7.72	97.87	111.00
1	E	31	ARG	NE-CZ-NH1	-7.71	116.44	120.30
2	B	440	ARG	CB-CG-CD	-7.69	91.60	111.60
2	L	407	ARG	NE-CZ-NH2	-7.68	116.46	120.30
2	B	505	ILE	CG1-CB-CG2	-7.67	94.53	111.40
2	D	313	ARG	NE-CZ-NH1	7.67	124.14	120.30
1	C	170	LEU	CB-CG-CD1	-7.65	98.00	111.00
2	L	409	ARG	NE-CZ-NH2	7.63	124.12	120.30
2	H	364	LEU	CB-CG-CD2	-7.62	98.04	111.00
2	H	428	ARG	NE-CZ-NH1	7.61	124.11	120.30
2	D	414	ARG	NE-CZ-NH1	7.61	124.11	120.30
1	C	78	GLU	OE1-CD-OE2	7.61	132.43	123.30
2	D	386	ASP	CB-CG-OD2	7.60	125.14	118.30
1	G	52	LEU	CA-CB-CG	7.59	132.76	115.30
1	I	50	LEU	CB-CG-CD1	-7.57	98.13	111.00
2	B	416	LEU	CA-CB-CG	7.57	132.70	115.30
1	K	142	ARG	NE-CZ-NH1	7.57	124.08	120.30
1	A	175	CYS	CA-CB-SG	7.55	127.59	114.00
2	J	524	ASP	CB-CG-OD2	-7.54	111.51	118.30
2	B	365	LEU	CB-CG-CD1	-7.54	98.19	111.00
2	L	457	ARG	NE-CZ-NH2	-7.53	116.53	120.30
1	I	176	GLU	OE1-CD-OE2	7.51	132.31	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	142	ARG	NE-CZ-NH2	7.48	124.04	120.30
1	E	130	LEU	CB-CG-CD1	7.48	123.71	111.00
2	D	333	ARG	CG-CD-NE	-7.47	96.10	111.80
1	E	68	LEU	CB-CG-CD2	-7.47	98.29	111.00
2	J	473	LYS	CD-CE-NZ	-7.38	94.73	111.70
1	E	154	LYS	CD-CE-NZ	7.35	128.61	111.70
2	B	377	ARG	NE-CZ-NH2	7.35	123.98	120.30
2	D	312	ASP	CB-CG-OD1	7.35	124.91	118.30
1	G	35	ILE	CG1-CB-CG2	-7.31	95.31	111.40
2	H	522	ARG	NE-CZ-NH2	7.31	123.95	120.30
2	F	420	ASP	CB-CG-OD1	7.30	124.87	118.30
1	C	180	LYS	CB-CA-C	7.30	125.00	110.40
2	J	524	ASP	CB-CG-OD1	7.30	124.87	118.30
1	A	167	ARG	NE-CZ-NH1	-7.29	116.66	120.30
2	H	428	ARG	NE-CZ-NH2	-7.28	116.66	120.30
2	H	499	GLU	OE1-CD-OE2	7.26	132.01	123.30
1	E	174	ARG	NE-CZ-NH1	-7.23	116.68	120.30
2	D	384	VAL	CG1-CB-CG2	-7.23	99.34	110.90
1	E	74	ASP	CB-CG-OD1	7.22	124.80	118.30
2	J	312	ASP	CB-CG-OD2	-7.22	111.81	118.30
2	J	434	ASP	OD1-CG-OD2	7.20	136.99	123.30
2	J	363	LEU	CB-CG-CD2	-7.19	98.78	111.00
2	J	440	ARG	CB-CG-CD	-7.16	92.98	111.60
2	B	507	LYS	CD-CE-NZ	7.16	128.17	111.70
2	H	537	ASN	C-N-CA	7.14	139.55	121.70
1	A	184	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	E	113	VAL	CG1-CB-CG2	-7.13	99.49	110.90
2	B	510	MET	CA-CB-CG	7.09	125.35	113.30
2	L	440	ARG	CB-CG-CD	-7.08	93.20	111.60
1	K	106	LEU	CA-CB-CG	7.06	131.53	115.30
1	K	168	GLU	OE1-CD-OE2	7.04	131.75	123.30
2	B	330	ARG	NE-CZ-NH1	7.02	123.81	120.30
1	K	85	LEU	CB-CG-CD1	-7.01	99.08	111.00
1	I	21	LEU	CB-CG-CD1	-7.01	99.08	111.00
2	B	409	ARG	NE-CZ-NH1	-6.98	116.81	120.30
1	C	81	ASP	CB-CG-OD1	6.98	124.58	118.30
1	G	74	ASP	CB-CG-OD1	6.96	124.56	118.30
1	A	167	ARG	NE-CZ-NH2	6.95	123.78	120.30
1	C	126	ILE	CA-CB-CG1	-6.94	97.81	111.00
2	J	531	ARG	NE-CZ-NH1	-6.94	116.83	120.30
2	D	376	GLU	OE1-CD-OE2	6.94	131.62	123.30
2	B	483	ASP	CB-CG-OD1	6.93	124.54	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	183	TYR	CZ-CE2-CD2	-6.93	113.56	119.80
1	E	81	ASP	CB-CG-OD1	6.91	124.52	118.30
1	C	102	GLY	CA-C-O	6.89	133.00	120.60
1	A	39	LEU	CB-CG-CD2	-6.83	99.38	111.00
2	J	438	SER	N-CA-CB	6.81	120.71	110.50
2	D	321	THR	N-CA-C	-6.79	92.68	111.00
2	D	419	LEU	CA-CB-CG	-6.77	99.73	115.30
2	B	307	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	A	32	ASP	CB-CG-OD2	-6.76	112.22	118.30
2	D	362	ASP	CB-CG-OD2	6.73	124.36	118.30
1	G	86	GLU	OE1-CD-OE2	6.72	131.36	123.30
1	C	69	GLU	OE1-CD-OE2	-6.71	115.24	123.30
1	C	189	ILE	CG1-CB-CG2	-6.71	96.65	111.40
2	J	451	ASN	N-CA-C	-6.71	92.89	111.00
2	L	434	ASP	CB-CG-OD2	-6.70	112.27	118.30
1	A	94	ARG	CD-NE-CZ	6.70	132.97	123.60
1	C	57	ASP	CB-CG-OD1	6.68	124.31	118.30
1	E	85	LEU	CB-CG-CD1	-6.68	99.65	111.00
2	J	386	ASP	CB-CG-OD1	-6.68	112.29	118.30
1	E	52	LEU	CA-CB-CG	6.67	130.64	115.30
1	E	167	ARG	NE-CZ-NH1	-6.67	116.97	120.30
2	D	336	LEU	CB-CG-CD2	-6.66	99.67	111.00
2	D	328	ILE	CG1-CB-CG2	-6.64	96.80	111.40
2	B	440	ARG	NE-CZ-NH1	6.63	123.61	120.30
2	J	409	ARG	NE-CZ-NH2	-6.63	116.99	120.30
1	E	21	LEU	N-CA-C	6.62	128.88	111.00
2	J	457	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	K	40	ALA	CA-C-N	-6.61	102.67	117.20
2	B	362	ASP	CB-CG-OD2	6.60	124.24	118.30
2	D	420	ASP	CB-CG-OD2	-6.58	112.38	118.30
1	G	126	ILE	CG1-CB-CG2	-6.58	96.93	111.40
1	E	171	ILE	CG1-CB-CG2	-6.57	96.94	111.40
1	A	174	ARG	NE-CZ-NH1	6.57	123.58	120.30
2	H	434	ASP	N-CA-CB	-6.55	98.80	110.60
2	J	414	ARG	CD-NE-CZ	6.55	132.78	123.60
2	B	538	CYS	N-CA-C	6.54	128.65	111.00
2	F	434	ASP	CB-CG-OD1	-6.54	112.42	118.30
1	I	81	ASP	CB-CG-OD2	-6.52	112.43	118.30
1	I	166	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	K	121	PRO	CA-C-N	-6.52	102.85	117.20
1	G	106	LEU	CA-CB-CG	6.51	130.28	115.30
1	G	147	ASP	CB-CG-OD1	6.51	124.16	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	447	TYR	CB-CG-CD2	-6.49	117.10	121.00
2	J	478	LEU	CA-CB-CG	6.49	130.22	115.30
1	E	160	LEU	CA-CB-CG	-6.47	100.42	115.30
2	D	333	ARG	NH1-CZ-NH2	6.47	126.51	119.40
2	H	517	ASP	CB-CG-OD2	-6.46	112.48	118.30
1	K	74	ASP	CB-CG-OD2	-6.46	112.49	118.30
2	H	478	LEU	CB-CG-CD1	-6.45	100.03	111.00
2	J	426	VAL	CG1-CB-CG2	6.44	121.21	110.90
2	F	426	VAL	CB-CA-C	-6.44	99.17	111.40
2	J	337	VAL	CG1-CB-CG2	6.42	121.17	110.90
2	J	457	ARG	NE-CZ-NH1	6.41	123.51	120.30
1	I	24	GLU	OE1-CD-OE2	6.41	130.99	123.30
2	L	428	ARG	CD-NE-CZ	6.41	132.57	123.60
2	H	378	ILE	CG1-CB-CG2	-6.40	97.32	111.40
2	L	522	ARG	NE-CZ-NH2	6.39	123.50	120.30
1	C	94	ARG	CD-NE-CZ	6.38	132.54	123.60
1	G	167	ARG	NE-CZ-NH1	6.38	123.49	120.30
2	D	428	ARG	CB-CG-CD	6.38	128.19	111.60
2	L	413	ASP	CB-CG-OD2	6.37	124.03	118.30
1	I	199	ASP	CB-CG-OD2	6.36	124.02	118.30
2	B	407	ARG	NE-CZ-NH1	6.35	123.47	120.30
1	G	70	VAL	CG1-CB-CG2	-6.35	100.74	110.90
1	K	68	LEU	CB-CG-CD1	6.35	121.80	111.00
2	H	442	ILE	CB-CG1-CD1	-6.34	96.14	113.90
1	A	81	ASP	CB-CG-OD1	6.33	124.00	118.30
2	F	457	ARG	NH1-CZ-NH2	6.31	126.34	119.40
1	C	184	ARG	CG-CD-NE	-6.30	98.58	111.80
1	A	38	ARG	NE-CZ-NH2	-6.29	117.15	120.30
2	H	519	LEU	CB-CG-CD1	-6.29	100.30	111.00
2	D	318	LYS	CA-CB-CG	6.29	127.24	113.40
2	D	337	VAL	CG1-CB-CG2	6.28	120.95	110.90
2	H	330	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	K	43	ASP	CB-CG-OD2	-6.27	112.66	118.30
2	B	430	LEU	CA-CB-CG	6.27	129.72	115.30
2	J	522	ARG	NE-CZ-NH1	-6.26	117.17	120.30
1	K	32	ASP	CB-CG-OD2	-6.25	112.67	118.30
1	E	66	SER	N-CA-CB	-6.25	101.12	110.50
2	D	428	ARG	CD-NE-CZ	6.23	132.32	123.60
1	E	184	ARG	NE-CZ-NH2	-6.23	117.19	120.30
2	F	474	LEU	CB-CG-CD2	-6.22	100.43	111.00
2	J	450	ARG	NE-CZ-NH2	6.18	123.39	120.30
2	F	414	ARG	CD-NE-CZ	6.18	132.25	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	94	ARG	N-CA-CB	6.16	121.69	110.60
1	A	130	LEU	CB-CG-CD1	6.14	121.44	111.00
2	D	528	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	I	57	ASP	CB-CG-OD2	-6.14	112.78	118.30
1	E	21	LEU	CA-CB-CG	6.13	129.41	115.30
2	B	360	ASP	CB-CG-OD1	6.13	123.82	118.30
2	H	369	ASN	CB-CA-C	6.13	122.66	110.40
2	H	369	ASN	CA-C-N	-6.13	103.95	116.20
2	J	426	VAL	CB-CA-C	-6.11	99.78	111.40
1	G	37	ASN	N-CA-C	6.11	127.50	111.00
2	D	507	LYS	CD-CE-NZ	6.10	125.73	111.70
1	G	103	GLU	CB-CA-C	-6.09	98.21	110.40
2	H	519	LEU	CB-CG-CD2	6.09	121.36	111.00
2	J	416	LEU	CA-CB-CG	6.09	129.31	115.30
1	E	157	VAL	CG1-CB-CG2	-6.09	101.16	110.90
1	A	122	MET	CG-SD-CE	6.07	109.92	100.20
2	H	414	ARG	CD-NE-CZ	6.07	132.10	123.60
1	K	139	LEU	CB-CG-CD2	-6.07	100.68	111.00
1	G	16	TYR	CD1-CE1-CZ	-6.06	114.34	119.80
1	I	174	ARG	NE-CZ-NH1	-6.06	117.27	120.30
1	I	174	ARG	CG-CD-NE	-6.06	99.08	111.80
1	C	65	ASP	CB-CG-OD1	6.05	123.75	118.30
1	A	168	GLU	OE1-CD-OE2	6.04	130.55	123.30
1	K	106	LEU	CB-CG-CD2	-6.03	100.75	111.00
1	E	168	GLU	CB-CG-CD	-6.00	98.00	114.20
1	K	178	ASP	CB-CG-OD2	-6.00	112.90	118.30
1	C	37	ASN	N-CA-C	5.99	127.17	111.00
1	G	106	LEU	CB-CG-CD1	5.98	121.17	111.00
2	J	440	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	K	31	ARG	NE-CZ-NH2	5.98	123.29	120.30
2	F	531	ARG	NE-CZ-NH2	-5.97	117.31	120.30
2	L	457	ARG	CB-CA-C	-5.97	98.47	110.40
2	L	307	ARG	NE-CZ-NH1	5.94	123.27	120.30
2	B	322	PRO	N-CA-C	5.92	127.49	112.10
2	D	450	ARG	CG-CD-NE	-5.92	99.37	111.80
2	F	383	ARG	NE-CZ-NH2	-5.92	117.34	120.30
2	L	383	ARG	CG-CD-NE	-5.90	99.40	111.80
2	D	323	ASP	CB-CG-OD1	5.89	123.60	118.30
1	G	158	LEU	CA-CB-CG	5.89	128.85	115.30
2	H	372	LEU	CB-CG-CD1	5.88	120.99	111.00
1	K	120	VAL	CB-CA-C	-5.88	100.23	111.40
2	J	360	ASP	CB-CG-OD2	-5.87	113.01	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	536	GLU	OE1-CD-OE2	5.87	130.35	123.30
1	K	150	GLN	N-CA-CB	5.87	121.17	110.60
2	J	311	ARG	NE-CZ-NH2	-5.87	117.37	120.30
2	J	321	THR	N-CA-C	-5.87	95.16	111.00
2	B	396	LEU	CB-CG-CD2	5.85	120.95	111.00
1	K	199	ASP	CB-CG-OD2	5.85	123.57	118.30
2	F	336	LEU	CB-CG-CD2	-5.85	101.06	111.00
2	D	369	ASN	CB-CA-C	5.85	122.09	110.40
2	D	365	LEU	CB-CG-CD2	5.84	120.93	111.00
2	J	443	LYS	CD-CE-NZ	5.82	125.08	111.70
2	H	428	ARG	CD-NE-CZ	5.81	131.74	123.60
1	A	94	ARG	CB-CG-CD	5.81	126.71	111.60
1	C	154	LYS	CB-CA-C	-5.81	98.79	110.40
2	L	473	LYS	CG-CD-CE	-5.81	94.48	111.90
2	B	457	ARG	CB-CA-C	-5.80	98.79	110.40
1	C	101	ALA	CA-C-O	-5.80	107.92	120.10
1	A	147	ASP	CB-CG-OD2	-5.79	113.09	118.30
1	E	3	GLU	CB-CA-C	-5.79	98.81	110.40
1	G	183	TYR	CB-CG-CD1	-5.79	117.53	121.00
1	K	86	GLU	OE1-CD-OE2	5.79	130.25	123.30
1	A	101	ALA	CA-C-O	-5.78	107.96	120.10
1	C	178	ASP	CB-CG-OD2	-5.78	113.10	118.30
2	F	330	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	C	137	ILE	CG1-CB-CG2	5.76	124.08	111.40
2	D	336	LEU	CB-CG-CD1	5.75	120.78	111.00
1	G	103	GLU	OE1-CD-OE2	5.75	130.20	123.30
1	K	121	PRO	O-C-N	5.75	131.90	122.70
1	A	94	ARG	CA-CB-CG	5.75	126.05	113.40
2	J	360	ASP	CB-CG-OD1	5.75	123.47	118.30
1	E	160	LEU	CB-CG-CD1	-5.74	101.23	111.00
1	E	142	ARG	NH1-CZ-NH2	-5.74	113.08	119.40
2	B	537	ASN	C-N-CA	5.74	136.04	121.70
2	J	383	ARG	NE-CZ-NH1	-5.73	117.44	120.30
1	I	32	ASP	CB-CA-C	-5.73	98.95	110.40
2	L	442	ILE	CG1-CB-CG2	5.73	124.00	111.40
2	J	368	ASN	N-CA-CB	5.72	120.91	110.60
1	I	69	GLU	OE1-CD-OE2	-5.71	116.44	123.30
2	J	497	ASN	N-CA-CB	-5.71	100.33	110.60
2	L	333	ARG	NH1-CZ-NH2	5.70	125.67	119.40
2	J	519	LEU	CA-CB-CG	-5.70	102.20	115.30
2	J	312	ASP	CB-CG-OD1	5.70	123.43	118.30
1	C	160	LEU	CB-CG-CD2	-5.69	101.33	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	158	LEU	CB-CG-CD2	-5.68	101.34	111.00
2	L	507	LYS	CD-CE-NZ	5.67	124.75	111.70
1	E	182	ALA	CB-CA-C	-5.66	101.61	110.10
2	B	452	GLY	N-CA-C	-5.66	98.96	113.10
2	J	386	ASP	CB-CG-OD2	5.65	123.39	118.30
1	C	168	GLU	N-CA-C	5.65	126.25	111.00
2	J	407	ARG	CG-CD-NE	-5.65	99.94	111.80
2	L	461	ILE	CG1-CB-CG2	-5.65	98.98	111.40
1	A	178	ASP	CB-CG-OD2	5.64	123.38	118.30
2	B	504	LEU	CD1-CG-CD2	-5.64	93.58	110.50
2	L	414	ARG	CD-NE-CZ	5.64	131.50	123.60
2	H	470	ILE	CG1-CB-CG2	-5.64	99.00	111.40
1	G	142	ARG	NE-CZ-NH2	-5.63	117.48	120.30
2	L	311	ARG	CB-CA-C	-5.63	99.13	110.40
2	F	457	ARG	NE-CZ-NH1	-5.63	117.48	120.30
1	A	86	GLU	OE1-CD-OE2	5.63	130.06	123.30
1	K	65	ASP	CB-CG-OD2	-5.63	113.24	118.30
2	J	464	GLY	N-CA-C	-5.61	99.07	113.10
1	C	47	GLU	OE1-CD-OE2	5.60	130.02	123.30
2	L	309	VAL	CG1-CB-CG2	5.59	119.84	110.90
1	K	180	LYS	CD-CE-NZ	5.59	124.55	111.70
2	B	420	ASP	CB-CG-OD2	-5.58	113.27	118.30
2	H	493	LYS	CD-CE-NZ	5.58	124.55	111.70
1	K	52	LEU	CA-CB-CG	5.58	128.13	115.30
1	C	22	ALA	N-CA-C	-5.57	95.95	111.00
2	F	365	LEU	CA-CB-CG	5.57	128.12	115.30
2	B	414	ARG	NE-CZ-NH2	5.57	123.09	120.30
1	G	106	LEU	CB-CG-CD2	-5.57	101.53	111.00
2	J	428	ARG	CD-NE-CZ	5.57	131.40	123.60
2	F	492	VAL	CG1-CB-CG2	5.57	119.81	110.90
1	G	78	GLU	OE1-CD-OE2	5.57	129.98	123.30
2	H	455	ASP	CB-CG-OD2	5.56	123.31	118.30
1	A	199	ASP	CB-CG-OD2	5.55	123.30	118.30
1	I	37	ASN	N-CA-C	5.55	125.99	111.00
1	E	128	ILE	CG1-CB-CG2	-5.54	99.20	111.40
2	B	390	LYS	CD-CE-NZ	-5.54	98.96	111.70
2	F	450	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	I	196	VAL	CA-CB-CG2	-5.54	102.60	110.90
1	C	51	LEU	CB-CG-CD2	-5.53	101.60	111.00
2	J	307	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	A	94	ARG	CG-CD-NE	-5.53	100.19	111.80
2	D	368	ASN	CA-C-N	-5.53	105.04	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	369	ASN	CA-C-N	-5.52	105.15	116.20
2	B	398	GLU	CG-CD-OE1	5.52	129.34	118.30
2	D	428	ARG	N-CA-CB	5.51	120.51	110.60
2	H	483	ASP	CB-CG-OD1	5.51	123.26	118.30
2	H	524	ASP	CB-CG-OD1	-5.50	113.35	118.30
1	A	100	ASP	C-N-CA	5.49	135.42	121.70
1	K	37	ASN	N-CA-C	5.49	125.81	111.00
1	K	1	PRO	N-CA-CB	5.48	109.88	103.30
1	C	176	GLU	OE1-CD-OE2	5.48	129.87	123.30
1	A	43	ASP	CB-CG-OD2	-5.48	113.37	118.30
1	C	166	ARG	CD-NE-CZ	5.47	131.26	123.60
1	A	62	LEU	CA-CB-CG	5.46	127.85	115.30
2	B	326	THR	OG1-CB-CG2	-5.46	97.45	110.00
2	H	482	GLY	N-CA-C	5.46	126.74	113.10
1	C	50	LEU	CB-CG-CD2	-5.45	101.74	111.00
2	H	411	LYS	CB-CA-C	-5.45	99.51	110.40
1	I	165	GLN	CA-CB-CG	5.45	125.38	113.40
1	A	103	GLU	CB-CA-C	-5.44	99.51	110.40
2	L	528	ARG	NE-CZ-NH2	5.44	123.02	120.30
2	J	368	ASN	CA-C-N	-5.42	105.28	117.20
1	K	191	GLY	N-CA-C	5.41	126.63	113.10
1	A	5	LEU	CB-CA-C	-5.41	99.92	110.20
1	I	81	ASP	CB-CG-OD1	5.40	123.16	118.30
2	L	383	ARG	NE-CZ-NH1	-5.40	117.60	120.30
1	K	114	VAL	CG1-CB-CG2	-5.40	102.26	110.90
2	F	409	ARG	NE-CZ-NH2	5.39	123.00	120.30
1	K	38	ARG	NE-CZ-NH2	5.38	122.99	120.30
1	K	165	GLN	CA-CB-CG	5.38	125.22	113.40
1	E	188	ARG	N-CA-CB	5.37	120.27	110.60
1	G	51	LEU	CB-CG-CD2	-5.37	101.87	111.00
1	K	51	LEU	CB-CG-CD2	-5.37	101.87	111.00
2	J	434	ASP	CB-CG-OD2	-5.37	113.47	118.30
1	I	168	GLU	OE1-CD-OE2	5.36	129.74	123.30
2	B	383	ARG	NE-CZ-NH2	-5.36	117.62	120.30
2	D	451	ASN	N-CA-C	-5.36	96.54	111.00
2	L	426	VAL	CG1-CB-CG2	-5.34	102.35	110.90
2	B	384	VAL	CB-CA-C	-5.34	101.25	111.40
2	D	369	ASN	CA-C-N	-5.33	105.53	116.20
2	H	383	ARG	NH1-CZ-NH2	5.32	125.25	119.40
2	B	434	ASP	OD1-CG-OD2	5.32	133.40	123.30
2	J	507	LYS	CD-CE-NZ	5.31	123.92	111.70
1	C	85	LEU	CB-CG-CD1	-5.31	101.97	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	148	GLU	CG-CD-OE2	-5.31	107.68	118.30
1	A	41	LYS	CD-CE-NZ	-5.30	99.51	111.70
2	H	325	LYS	CD-CE-NZ	-5.30	99.51	111.70
1	G	154	LYS	CA-CB-CG	5.29	125.05	113.40
2	F	328	ILE	CG1-CB-CG2	-5.29	99.76	111.40
1	G	9	PRO	N-CD-CG	-5.29	95.27	103.20
1	K	148	GLU	CG-CD-OE2	-5.28	107.73	118.30
1	C	129	SER	N-CA-CB	5.28	118.42	110.50
2	L	434	ASP	OD1-CG-OD2	5.28	133.34	123.30
1	I	21	LEU	CB-CG-CD2	5.27	119.96	111.00
2	L	390	LYS	CD-CE-NZ	-5.26	99.59	111.70
1	G	176	GLU	OE1-CD-OE2	5.25	129.60	123.30
1	G	74	ASP	CB-CG-OD2	-5.25	113.57	118.30
2	L	307	ARG	NE-CZ-NH2	-5.25	117.68	120.30
2	B	413	ASP	CB-CA-C	5.25	120.89	110.40
1	A	35	ILE	CG1-CB-CG2	-5.24	99.87	111.40
1	I	83	TYR	CD1-CE1-CZ	5.24	124.52	119.80
2	F	447	TYR	CB-CG-CD2	-5.24	117.86	121.00
2	L	447	TYR	CB-CG-CD2	-5.23	117.86	121.00
2	F	428	ARG	CD-NE-CZ	5.23	130.92	123.60
2	D	392	VAL	CA-CB-CG2	5.23	118.74	110.90
1	I	68	LEU	CB-CG-CD2	-5.22	102.12	111.00
1	I	176	GLU	CG-CD-OE2	-5.22	107.86	118.30
2	B	365	LEU	CB-CG-CD2	5.20	119.84	111.00
1	I	35	ILE	CG1-CB-CG2	-5.20	99.96	111.40
2	H	457	ARG	NH1-CZ-NH2	-5.19	113.69	119.40
2	B	386	ASP	CB-CG-OD1	-5.17	113.64	118.30
1	E	101	ALA	CA-C-O	-5.17	109.24	120.10
2	J	447	TYR	OH-CZ-CE2	-5.17	106.14	120.10
2	J	508	LEU	CB-CG-CD2	-5.17	102.21	111.00
2	F	312	ASP	CB-CG-OD1	5.17	122.95	118.30
2	J	505	ILE	CG1-CB-CG2	-5.16	100.04	111.40
1	A	23	LEU	CB-CG-CD2	-5.16	102.23	111.00
1	I	74	ASP	CB-CG-OD1	5.16	122.94	118.30
1	E	22	ALA	N-CA-C	-5.16	97.08	111.00
1	G	192	GLU	OE1-CD-OE2	5.16	129.49	123.30
1	C	101	ALA	CA-C-N	5.15	126.51	116.20
1	E	154	LYS	CA-CB-CG	5.15	124.73	113.40
1	C	154	LYS	CA-CB-CG	5.15	124.72	113.40
1	A	135	ILE	CG1-CB-CG2	-5.14	100.09	111.40
1	C	176	GLU	CG-CD-OE2	-5.14	108.02	118.30
2	D	416	LEU	CA-CB-CG	5.14	127.12	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	81	ASP	CB-CG-OD2	-5.13	113.68	118.30
1	I	137	ILE	CG1-CB-CG2	5.13	122.70	111.40
1	K	102	GLY	C-N-CA	5.13	134.52	121.70
2	D	348	GLY	N-CA-C	-5.13	100.28	113.10
2	J	461	ILE	CB-CA-C	-5.12	101.36	111.60
2	B	411	LYS	CB-CA-C	-5.12	100.17	110.40
2	J	371	GLY	N-CA-C	5.12	125.89	113.10
1	I	78	GLU	CA-CB-CG	-5.11	102.15	113.40
1	K	170	LEU	CB-CG-CD2	5.11	119.69	111.00
1	C	94	ARG	CA-CB-CG	5.11	124.64	113.40
1	E	139	LEU	CB-CG-CD1	-5.11	102.32	111.00
2	L	312	ASP	CB-CG-OD1	5.10	122.89	118.30
2	D	333	ARG	CD-NE-CZ	5.10	130.74	123.60
1	E	180	LYS	CD-CE-NZ	5.10	123.43	111.70
2	H	324	TYR	N-CA-C	-5.10	97.24	111.00
1	C	103	GLU	N-CA-CB	-5.10	101.43	110.60
2	F	413	ASP	OD1-CG-OD2	-5.09	113.62	123.30
2	L	354	LEU	CB-CG-CD2	-5.09	102.35	111.00
2	L	336	LEU	CB-CG-CD1	-5.09	102.35	111.00
2	L	481	GLU	N-CA-CB	-5.08	101.45	110.60
2	B	386	ASP	CB-CG-OD2	5.08	122.87	118.30
1	E	37	ASN	N-CA-C	5.08	124.70	111.00
2	D	382	GLY	CA-C-O	5.07	129.73	120.60
2	L	461	ILE	N-CA-C	-5.07	97.31	111.00
2	H	503	GLN	N-CA-CB	-5.07	101.47	110.60
1	I	146	ASP	CB-CG-OD1	-5.07	113.74	118.30
2	H	426	VAL	CA-CB-CG2	-5.06	103.31	110.90
2	H	438	SER	N-CA-CB	5.05	118.08	110.50
2	H	332	PRO	CB-CA-C	-5.05	99.37	112.00
2	H	337	VAL	CG1-CB-CG2	5.05	118.98	110.90
2	H	523	PHE	CD1-CE1-CZ	-5.05	114.04	120.10
1	G	31	ARG	NE-CZ-NH1	-5.05	117.78	120.30
2	J	510	MET	CG-SD-CE	-5.05	92.12	100.20
2	B	522	ARG	NE-CZ-NH1	-5.05	117.78	120.30
2	H	414	ARG	NE-CZ-NH2	-5.04	117.78	120.30
2	H	426	VAL	CB-CA-C	-5.04	101.83	111.40
1	E	126	ILE	CB-CG1-CD1	-5.04	99.80	113.90
2	H	399	MET	CG-SD-CE	5.03	108.25	100.20
2	F	447	TYR	CD1-CE1-CZ	-5.03	115.27	119.80
2	L	458	PRO	CB-CA-C	-5.02	99.45	112.00
1	I	167	ARG	CD-NE-CZ	5.02	130.63	123.60
1	C	180	LYS	N-CA-C	-5.01	97.46	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	111	PRO	C-N-CA	-5.01	111.78	122.30
2	L	526	VAL	CB-CA-C	-5.00	101.89	111.40
1	E	43	ASP	CB-CG-OD1	-5.00	113.80	118.30

There are no chirality outliers.

All (75) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	16	TYR	Sidechain
1	A	18	HIS	Mainchain
1	A	35	ILE	Mainchain
1	A	56	TYR	Sidechain
2	B	324	TYR	Sidechain
2	B	422	ASN	Mainchain
2	B	436	TYR	Sidechain
2	B	440	ARG	Sidechain
2	B	455	ASP	Mainchain
2	B	457	ARG	Mainchain
2	B	495	ILE	Mainchain
2	B	521	TYR	Sidechain
2	B	537	ASN	Mainchain
1	C	131	PHE	Mainchain
1	C	171	ILE	Mainchain
1	C	180	LYS	Mainchain
1	C	182	ALA	Mainchain
1	C	67	PHE	Mainchain
1	C	83	TYR	Mainchain
1	C	99	PHE	Mainchain
2	D	330	ARG	Sidechain
2	D	332	PRO	Mainchain
2	D	353	HIS	Sidechain
2	D	359	HIS	Sidechain
2	D	381	ALA	Mainchain
2	D	513	ALA	Mainchain
1	E	162	GLU	Mainchain
1	E	175	CYS	Mainchain
1	E	184	ARG	Sidechain
1	E	56	TYR	Sidechain
1	E	67	PHE	Sidechain
2	F	330	ARG	Mainchain
2	F	353	HIS	Sidechain
2	F	366	ASN	Mainchain

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Mol	Chain	Res	Type	Group
2	F	407	ARG	Sidechain
2	F	437	TYR	Sidechain
2	F	460	HIS	Sidechain
1	G	12	THR	Mainchain
1	G	144	TYR	Sidechain
1	G	16	TYR	Sidechain
1	G	184	ARG	Sidechain
1	G	188	ARG	Sidechain
1	G	56	TYR	Sidechain
2	H	340	PRO	Mainchain
2	H	386	ASP	Mainchain
2	H	436	TYR	Sidechain
2	H	450	ARG	Mainchain
2	H	457	ARG	Sidechain
1	I	13	ALA	Mainchain
1	I	146	ASP	Mainchain
1	I	198	PHE	Mainchain
1	I	35	ILE	Mainchain
2	J	341	GLN	Mainchain
2	J	346	THR	Mainchain
2	J	363	LEU	Mainchain
2	J	385	VAL	Mainchain
2	J	407	ARG	Sidechain
2	J	460	HIS	Mainchain
2	J	479	TYR	Sidechain
2	J	521	TYR	Sidechain
1	K	100	ASP	Mainchain
1	K	132	ALA	Mainchain
1	K	182	ALA	Mainchain
1	K	19	ILE	Mainchain
1	K	39	LEU	Mainchain
1	K	56	TYR	Sidechain
1	K	64	ARG	Mainchain
1	K	79	TYR	Sidechain
1	K	99	PHE	Sidechain
2	L	342	SER	Mainchain
2	L	351	PHE	Mainchain
2	L	353	HIS	Sidechain
2	L	388	TYR	Sidechain
2	L	401	GLN	Mainchain
2	L	510	MET	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	33	0
1	C	1571	0	1499	30	0
1	E	1571	0	1499	33	0
1	G	1571	0	1499	32	1
1	I	1571	0	1499	27	0
1	K	1571	0	1499	37	0
2	B	1877	0	1823	43	0
2	D	1877	0	1822	43	0
2	F	1877	0	1822	52	0
2	H	1877	0	1823	52	0
2	J	1877	0	1822	58	0
2	L	1877	0	1822	54	0
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	A	11	0	4	6	0
4	D	11	0	4	1	0
4	F	11	0	4	1	0
4	H	11	0	4	6	0
4	J	11	0	4	3	0
4	L	11	0	4	3	0
5	A	47	0	0	0	0
5	B	83	0	0	1	0
5	C	45	0	0	0	0
5	D	87	0	0	2	0
5	E	49	0	0	0	1
5	F	82	0	0	2	0
5	G	49	0	0	0	0
5	H	83	0	0	2	0
5	I	46	0	0	0	0
5	J	85	0	0	6	0
5	K	43	0	0	0	0
5	L	87	0	0	2	0
All	All	21546	0	19952	457	1

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 11.

All (457) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:ALA:CB	1:A:101:ALA:CA	1.77	1.62
2:B:507:LYS:CE	2:B:507:LYS:CD	1.78	1.62
1:E:154:LYS:CE	1:E:154:LYS:CD	1.76	1.61
2:F:532:LYS:CB	2:F:532:LYS:CA	1.76	1.61
2:J:390:LYS:CE	2:J:390:LYS:CD	1.77	1.60
2:H:414:ARG:CB	2:H:414:ARG:CG	1.76	1.60
2:F:303:GLN:CA	2:F:303:GLN:CB	1.80	1.60
2:J:507:LYS:CE	2:J:507:LYS:CD	1.76	1.59
1:C:180:LYS:CD	1:C:180:LYS:CG	1.78	1.59
2:J:390:LYS:CD	2:J:390:LYS:CG	1.80	1.58
1:G:154:LYS:CE	1:G:154:LYS:CD	1.78	1.58
2:J:532:LYS:CB	2:J:532:LYS:CA	1.76	1.58
2:J:303:GLN:CA	2:J:303:GLN:CB	1.82	1.57
2:L:429:CME:CZ	2:L:429:CME:CE	1.77	1.57
2:F:411:LYS:CD	2:F:411:LYS:CG	1.76	1.57
2:F:507:LYS:CE	2:F:507:LYS:CD	1.75	1.57
2:F:507:LYS:NZ	2:F:507:LYS:CE	1.68	1.57
1:G:180:LYS:CE	1:G:180:LYS:NZ	1.67	1.57
2:J:426:VAL:CG1	2:J:426:VAL:CB	1.75	1.56
2:B:339:ILE:CD1	2:B:339:ILE:CG1	1.80	1.56
1:C:180:LYS:NZ	1:C:180:LYS:CE	1.67	1.55
2:F:390:LYS:CE	2:F:390:LYS:CD	1.74	1.55
2:D:303:GLN:CB	2:D:303:GLN:CA	1.80	1.54
2:D:390:LYS:CD	2:D:390:LYS:CE	1.77	1.54
1:A:163:GLN:CD	1:A:163:GLN:CG	1.74	1.54
2:B:390:LYS:CD	2:B:390:LYS:CE	1.75	1.54
2:H:318:LYS:CE	2:H:318:LYS:NZ	1.67	1.54
2:H:429:CME:CE	2:H:429:CME:CZ	1.79	1.54
2:B:473:LYS:CE	2:B:473:LYS:NZ	1.70	1.54
2:L:303:GLN:CB	2:L:303:GLN:CA	1.79	1.54
2:J:507:LYS:CE	2:J:507:LYS:NZ	1.68	1.53
2:D:390:LYS:CG	2:D:390:LYS:CD	1.78	1.53
1:E:19:ILE:CG1	1:E:19:ILE:CD1	1.79	1.53
2:H:303:GLN:CA	2:H:303:GLN:CB	1.84	1.53
2:B:303:GLN:CA	2:B:303:GLN:CB	1.82	1.52
1:C:154:LYS:NZ	1:C:154:LYS:CE	1.68	1.51
1:C:100:ASP:CB	1:C:100:ASP:CG	1.75	1.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:154:LYS:CE	1:G:154:LYS:NZ	1.70	1.50
1:K:180:LYS:NZ	1:K:180:LYS:CE	1.68	1.50
1:E:154:LYS:CE	1:E:154:LYS:NZ	1.73	1.49
2:L:532:LYS:CA	2:L:532:LYS:CB	1.90	1.49
2:B:318:LYS:CE	2:B:318:LYS:NZ	1.73	1.48
2:D:516:MET:CE	2:D:516:MET:SD	2.01	1.48
2:D:507:LYS:CE	2:D:507:LYS:NZ	1.78	1.46
2:L:507:LYS:NZ	2:L:507:LYS:CE	1.77	1.46
1:K:175:CYS:SG	1:K:175:CYS:CB	2.04	1.45
2:H:507:LYS:CE	2:H:507:LYS:NZ	1.84	1.39
2:L:516:MET:SD	2:L:516:MET:CE	2.10	1.37
1:I:165:GLN:H	1:I:165:GLN:NE2	1.41	1.19
1:I:165:GLN:N	1:I:165:GLN:HE21	1.49	1.11
2:B:473:LYS:CD	2:B:473:LYS:NZ	2.20	1.03
2:L:416:LEU:H	2:L:416:LEU:HD23	1.23	1.03
1:K:165:GLN:NE2	1:K:165:GLN:H	1.59	1.01
1:A:165:GLN:H	1:A:165:GLN:NE2	1.61	0.98
2:F:416:LEU:H	2:F:416:LEU:HD23	1.28	0.97
1:C:165:GLN:H	1:C:165:GLN:HE21	1.02	0.97
2:H:416:LEU:H	2:H:416:LEU:HD23	1.30	0.96
2:J:368:ASN:ND2	2:J:371:GLY:H	1.66	0.92
2:B:497:ASN:HD22	2:B:499:GLU:H	1.16	0.89
1:E:165:GLN:NE2	1:E:165:GLN:H	1.71	0.88
2:B:364:LEU:HD22	2:B:440:ARG:HD3	1.55	0.88
2:L:497:ASN:ND2	2:L:499:GLU:H	1.72	0.88
2:J:408:HIS:NE2	5:J:4901:HOH:O	2.07	0.87
1:C:165:GLN:H	1:C:165:GLN:NE2	1.70	0.87
1:K:15:PRO:HD3	4:L:5550:DHB:C1	2.05	0.86
2:D:497:ASN:ND2	2:D:499:GLU:H	1.73	0.86
2:D:368:ASN:HD22	2:D:371:GLY:H	1.19	0.84
2:F:368:ASN:ND2	2:F:371:GLY:H	1.75	0.84
2:H:453:PRO:HB2	2:J:310:ILE:HD12	1.56	0.83
2:L:364:LEU:HD22	2:L:440:ARG:HD3	1.59	0.83
1:A:20:GLY:HA2	2:B:426:VAL:HG13	1.61	0.82
2:H:361:HIS:CD2	2:H:361:HIS:H	1.94	0.82
2:B:497:ASN:ND2	2:B:499:GLU:H	1.77	0.81
2:J:368:ASN:ND2	2:J:371:GLY:N	2.28	0.81
2:H:369:ASN:H	2:H:422:ASN:HD22	1.28	0.81
1:A:165:GLN:H	1:A:165:GLN:HE21	1.27	0.81
1:E:165:GLN:H	1:E:165:GLN:HE21	1.25	0.81
1:G:67:PHE:CZ	1:G:94:ARG:HD2	2.16	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:408:HIS:NE2	5:L:5901:HOH:O	2.14	0.80
2:B:473:LYS:HD3	2:B:473:LYS:NZ	1.95	0.80
2:D:368:ASN:ND2	2:D:371:GLY:H	1.80	0.80
2:J:390:LYS:HD3	5:J:4677:HOH:O	1.83	0.79
2:J:361:HIS:H	2:J:361:HIS:CD2	1.99	0.79
2:J:411:LYS:HZ2	2:J:411:LYS:H	1.31	0.76
2:L:497:ASN:HD22	2:L:499:GLU:H	1.32	0.76
2:H:411:LYS:HZ3	2:H:411:LYS:HB2	1.51	0.76
2:F:411:LYS:HZ2	2:F:411:LYS:H	1.34	0.76
2:J:426:VAL:CG1	2:J:426:VAL:HB	2.09	0.75
1:I:20:GLY:HA2	2:J:426:VAL:HG13	1.68	0.75
1:G:38:ARG:HG3	1:G:38:ARG:HH11	1.52	0.75
2:B:473:LYS:HD3	2:B:473:LYS:HZ2	1.52	0.74
2:J:368:ASN:HD21	2:J:371:GLY:N	1.84	0.74
1:E:31:ARG:HH12	2:F:428:ARG:HG2	1.52	0.73
2:F:361:HIS:CD2	2:F:361:HIS:H	2.05	0.73
2:B:390:LYS:NZ	2:B:390:LYS:CD	2.52	0.73
1:G:67:PHE:HZ	1:G:94:ARG:HD2	1.53	0.73
1:G:15:PRO:HD3	4:H:3550:DHB:C1	2.18	0.73
2:L:416:LEU:HD23	2:L:416:LEU:N	2.02	0.72
2:H:369:ASN:H	2:H:422:ASN:ND2	1.87	0.71
1:K:67:PHE:HZ	1:K:94:ARG:HD2	1.56	0.71
2:D:497:ASN:HD22	2:D:498:PRO:N	1.89	0.70
1:K:67:PHE:CZ	1:K:94:ARG:HD2	2.26	0.70
1:A:67:PHE:HZ	1:A:94:ARG:HD2	1.57	0.70
2:H:368:ASN:HD22	2:H:371:GLY:H	1.39	0.70
2:B:315:TRP:HZ2	2:B:503:GLN:NE2	1.90	0.70
1:C:98:THR:N	1:C:101:ALA:O	2.26	0.69
1:A:101:ALA:CB	1:A:101:ALA:C	2.61	0.69
1:K:165:GLN:HE21	1:K:165:GLN:H	1.40	0.69
2:D:411:LYS:NZ	2:D:411:LYS:HB2	2.07	0.69
1:E:25:ALA:HB1	1:E:98:THR:HG21	1.73	0.69
2:B:497:ASN:HD22	2:B:499:GLU:N	1.91	0.68
2:J:426:VAL:CG1	2:J:426:VAL:CA	2.69	0.68
1:E:19:ILE:CD1	1:E:19:ILE:HG21	2.24	0.68
2:L:361:HIS:H	2:L:361:HIS:CD2	2.10	0.68
2:H:416:LEU:N	2:H:416:LEU:HD23	2.07	0.68
1:K:69:GLU:OE1	1:K:94:ARG:HD3	1.95	0.67
1:E:19:ILE:CB	1:E:19:ILE:CD1	2.71	0.67
2:D:369:ASN:H	2:D:422:ASN:HD22	1.43	0.67
2:L:429:CME:CZ	2:L:429:CME:SD	2.83	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:PHE:CZ	1:A:94:ARG:HD2	2.30	0.66
2:L:497:ASN:HD22	2:L:499:GLU:N	1.93	0.66
1:A:15:PRO:HD3	4:A:550:DHB:C1	2.26	0.66
2:J:390:LYS:CD	2:J:390:LYS:CB	2.72	0.66
2:H:447:TYR:OH	4:H:3550:DHB:O4	2.14	0.66
2:H:318:LYS:NZ	2:H:318:LYS:CD	2.59	0.66
2:H:361:HIS:H	2:H:361:HIS:HD2	1.44	0.65
1:A:165:GLN:N	1:A:165:GLN:HE21	1.95	0.65
2:B:408:HIS:NE2	5:B:901:HOH:O	2.15	0.65
1:I:165:GLN:N	1:I:165:GLN:NE2	2.21	0.64
2:J:411:LYS:NZ	2:J:411:LYS:H	1.96	0.64
1:A:132:ALA:HB3	1:A:135:ILE:HD12	1.78	0.64
1:K:98:THR:N	1:K:101:ALA:O	2.27	0.64
2:J:368:ASN:HD22	2:J:371:GLY:H	1.45	0.64
2:F:359:HIS:O	2:F:366:ASN:HB3	1.98	0.64
1:I:165:GLN:H	1:I:165:GLN:HE21	0.73	0.64
2:L:364:LEU:HD22	2:L:440:ARG:CD	2.29	0.63
2:D:361:HIS:H	2:D:361:HIS:CD2	2.16	0.63
1:I:98:THR:N	1:I:101:ALA:O	2.28	0.63
1:E:31:ARG:NH1	2:F:428:ARG:HG2	2.13	0.63
2:F:507:LYS:CE	2:F:507:LYS:CG	2.72	0.63
1:E:19:ILE:CD1	1:E:19:ILE:CG2	2.77	0.63
1:G:80:GLN:O	1:G:91:SER:HB2	1.98	0.62
2:L:497:ASN:HD22	2:L:497:ASN:C	2.03	0.62
2:D:497:ASN:HD22	2:D:497:ASN:C	2.03	0.61
1:E:98:THR:N	1:E:101:ALA:O	2.30	0.61
1:K:25:ALA:HB1	1:K:98:THR:HG21	1.82	0.61
2:L:356:PHE:CE1	2:L:428:ARG:HD3	2.35	0.61
2:J:497:ASN:HD22	2:J:499:GLU:H	1.48	0.61
2:H:390:LYS:HD3	5:H:3677:HOH:O	2.01	0.61
2:B:473:LYS:CD	2:B:473:LYS:HZ2	2.05	0.60
2:D:411:LYS:HZ3	2:D:411:LYS:H	1.48	0.60
2:H:453:PRO:CB	2:J:310:ILE:HD12	2.30	0.60
1:A:15:PRO:HG3	1:A:133:ARG:HD2	1.83	0.60
1:G:70:VAL:HG11	1:G:106:LEU:HD21	1.83	0.60
2:B:361:HIS:CD2	2:B:361:HIS:H	2.20	0.59
2:D:497:ASN:HD22	2:D:499:GLU:H	1.50	0.59
2:B:507:LYS:CG	2:B:507:LYS:CE	2.77	0.59
2:L:497:ASN:ND2	2:L:499:GLU:N	2.47	0.59
2:H:497:ASN:HD22	2:H:499:GLU:H	1.49	0.59
2:F:497:ASN:ND2	2:F:499:GLU:H	2.01	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:15:PRO:HD3	4:L:5550:DHB:C6	2.34	0.58
1:G:155:CYS:HB3	1:G:158:LEU:HB2	1.85	0.58
2:B:369:ASN:H	2:B:422:ASN:HD22	1.51	0.58
1:A:101:ALA:CB	1:A:101:ALA:O	2.52	0.57
2:F:497:ASN:HD22	2:F:499:GLU:H	1.52	0.57
2:H:385:VAL:O	2:H:526:VAL:HA	2.04	0.57
2:H:368:ASN:ND2	2:H:371:GLY:H	2.01	0.57
2:F:416:LEU:N	2:F:416:LEU:HD23	2.10	0.57
1:K:143:LEU:C	1:K:143:LEU:HD23	2.24	0.57
2:F:409:ARG:HG3	2:F:409:ARG:NH1	2.20	0.57
2:J:497:ASN:ND2	2:J:499:GLU:H	2.03	0.57
1:E:19:ILE:HG21	1:E:19:ILE:HD13	1.87	0.56
1:E:15:PRO:HD3	4:F:2550:DHB:C1	2.35	0.56
2:F:478:LEU:C	2:F:478:LEU:HD23	2.26	0.56
1:K:143:LEU:HD23	1:K:144:TYR:N	2.20	0.56
2:J:447:TYR:OH	4:J:4550:DHB:O4	2.24	0.56
2:F:356:PHE:CD1	2:F:428:ARG:HD3	2.41	0.55
2:F:356:PHE:CE1	2:F:428:ARG:HD3	2.41	0.55
1:A:24:GLU:O	1:A:27:GLY:N	2.39	0.55
1:K:41:LYS:HB2	1:K:88:ALA:O	2.06	0.55
2:H:536:GLU:C	2:H:538:CYS:H	2.09	0.55
1:E:65:ASP:OD2	1:E:133:ARG:HD3	2.06	0.55
1:K:20:GLY:HA2	2:L:426:VAL:HG13	1.89	0.55
1:I:70:VAL:HG12	1:I:128:ILE:HG12	1.88	0.55
1:A:15:PRO:HD3	4:A:550:DHB:C6	2.37	0.54
1:G:165:GLN:HE21	1:G:165:GLN:H	1.54	0.54
2:B:497:ASN:ND2	2:B:499:GLU:N	2.53	0.54
1:I:161:ILE:O	1:I:167:ARG:NH2	2.41	0.54
1:C:20:GLY:HA2	2:D:426:VAL:HG13	1.89	0.54
2:J:376:GLU:O	2:J:442:ILE:HA	2.08	0.54
2:F:361:HIS:HD2	2:F:361:HIS:H	1.52	0.53
1:K:70:VAL:HG11	1:K:106:LEU:HD21	1.90	0.53
1:G:15:PRO:HD3	4:H:3550:DHB:C2	2.38	0.53
1:E:131:PHE:CD2	1:E:138:HIS:HB3	2.43	0.53
1:E:143:LEU:HD12	1:E:185:PHE:CD2	2.42	0.53
1:I:132:ALA:HB3	1:I:135:ILE:HD12	1.89	0.53
2:L:497:ASN:HD22	2:L:498:PRO:N	2.07	0.53
2:L:411:LYS:HZ3	2:L:411:LYS:H	1.57	0.53
1:A:15:PRO:CD	4:A:550:DHB:C6	2.87	0.53
2:F:315:TRP:HZ2	2:F:503:GLN:HE22	1.57	0.53
1:I:35:ILE:HG21	1:I:92:PHE:HE2	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:315:TRP:HZ2	2:B:503:GLN:HE21	1.56	0.52
1:I:133:ARG:HG3	2:J:326:THR:HG21	1.91	0.52
1:C:20:GLY:O	1:C:21:LEU:HD23	2.09	0.52
2:J:379:ILE:O	2:J:520:ALA:HA	2.09	0.52
1:K:145:PHE:CD1	1:K:145:PHE:N	2.77	0.52
2:L:483:ASP:HB3	2:L:486:ILE:HG13	1.91	0.52
2:J:453:PRO:HB2	2:L:310:ILE:HD12	1.91	0.52
2:D:368:ASN:HD22	2:D:371:GLY:N	1.99	0.52
1:I:65:ASP:OD2	1:I:133:ARG:HD3	2.10	0.52
2:J:376:GLU:OE1	2:J:443:LYS:HD3	2.09	0.52
2:H:361:HIS:CD2	2:H:361:HIS:N	2.69	0.52
1:I:162:GLU:O	1:I:164:PRO:HD3	2.09	0.52
1:C:15:PRO:HD3	4:D:1550:DHB:C1	2.39	0.52
2:L:368:ASN:ND2	2:L:371:GLY:H	2.08	0.52
2:B:305:ASN:O	2:B:533:THR:HG23	2.09	0.52
2:F:305:ASN:O	2:F:533:THR:HG23	2.10	0.52
2:D:369:ASN:H	2:D:422:ASN:ND2	2.06	0.52
2:F:416:LEU:CD2	2:F:416:LEU:H	2.12	0.51
2:F:449:TRP:N	2:F:449:TRP:CD1	2.77	0.51
1:I:165:GLN:CA	1:I:165:GLN:HE21	2.23	0.51
1:E:154:LYS:CE	1:E:154:LYS:CG	2.80	0.51
2:D:356:PHE:HZ	2:D:430:LEU:HD13	1.75	0.51
2:D:368:ASN:ND2	2:D:370:GLY:N	2.58	0.51
2:H:411:LYS:NZ	2:H:411:LYS:HB2	2.22	0.51
2:D:408:HIS:NE2	5:D:1901:HOH:O	2.14	0.51
2:D:390:LYS:HD3	5:D:1677:HOH:O	2.08	0.51
2:F:507:LYS:HE2	2:F:507:LYS:CD	2.19	0.51
2:L:408:HIS:CD2	5:L:5901:HOH:O	2.62	0.51
2:B:516:MET:SD	2:H:448:PRO:HB2	2.51	0.51
2:H:447:TYR:HB2	2:H:448:PRO:HD2	1.93	0.51
2:D:448:PRO:HD3	2:D:456:TRP:CZ3	2.46	0.51
2:D:368:ASN:ND2	2:D:370:GLY:H	2.08	0.50
2:H:507:LYS:O	2:H:521:TYR:HA	2.11	0.50
2:B:307:ARG:HG2	2:B:533:THR:HG22	1.93	0.50
2:J:416:LEU:H	2:J:416:LEU:HD23	1.77	0.50
1:G:31:ARG:NH1	2:H:428:ARG:HG2	2.26	0.50
2:F:409:ARG:HH11	2:F:409:ARG:HG3	1.77	0.50
2:J:484:PRO:O	2:J:487:PRO:HD2	2.12	0.50
2:D:303:GLN:CB	2:D:303:GLN:N	2.65	0.50
1:E:33:GLN:HG2	1:E:85:LEU:HD12	1.92	0.50
1:G:165:GLN:NE2	1:G:165:GLN:H	2.09	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:416:LEU:H	2:D:416:LEU:HD23	1.76	0.49
1:E:25:ALA:HB1	1:E:98:THR:CG2	2.41	0.49
1:G:132:ALA:O	1:G:135:ILE:HB	2.12	0.49
2:B:376:GLU:HG2	2:H:446:PRO:HD2	1.95	0.49
2:L:400:TRP:HA	2:L:425:GLY:O	2.12	0.49
2:H:495:ILE:HG21	2:H:500:ALA:HB3	1.94	0.49
1:K:147:ASP:OD2	1:K:174:ARG:NH1	2.46	0.48
1:K:15:PRO:CD	4:L:5550:DHB:C6	2.92	0.48
2:D:376:GLU:O	2:D:442:ILE:HA	2.13	0.48
2:J:497:ASN:C	2:J:497:ASN:HD22	2.16	0.48
2:F:478:LEU:O	2:F:478:LEU:HD23	2.13	0.48
2:H:411:LYS:HZ3	2:H:411:LYS:CB	2.21	0.48
1:E:160:LEU:HA	1:E:160:LEU:HD23	1.67	0.48
2:H:364:LEU:HD11	2:H:442:ILE:HG23	1.96	0.48
2:F:315:TRP:HZ2	2:F:503:GLN:NE2	2.11	0.48
1:C:16:TYR:HB3	1:C:19:ILE:HD13	1.95	0.48
1:G:143:LEU:HD23	1:G:143:LEU:C	2.33	0.48
2:J:382:GLY:HA2	2:J:522:ARG:HE	1.79	0.48
2:H:486:ILE:HG22	2:H:487:PRO:N	2.27	0.48
2:F:409:ARG:HH11	2:F:409:ARG:CG	2.26	0.48
1:E:164:PRO:HD2	1:E:165:GLN:HE22	1.79	0.47
2:J:408:HIS:CD2	5:J:4901:HOH:O	2.60	0.47
2:L:316:HIS:HB3	2:L:317:PRO:HD2	1.96	0.47
2:L:361:HIS:N	2:L:361:HIS:CD2	2.80	0.47
2:B:326:THR:HG22	2:B:330:ARG:HD2	1.96	0.47
2:L:356:PHE:HE1	2:L:428:ARG:HD3	1.79	0.47
1:K:160:LEU:HD11	2:L:340:PRO:HD3	1.96	0.47
1:G:110:LYS:NZ	1:G:147:ASP:OD1	2.36	0.47
2:L:356:PHE:CD1	2:L:428:ARG:HD3	2.50	0.47
1:C:25:ALA:C	1:C:27:GLY:H	2.16	0.47
1:G:14:GLY:HA2	4:H:3550:DHB:H2	1.96	0.47
1:I:123:ALA:O	1:I:124:PRO:C	2.53	0.47
1:I:67:PHE:HZ	1:I:94:ARG:HD2	1.78	0.47
2:D:497:ASN:C	2:D:497:ASN:ND2	2.68	0.47
1:A:15:PRO:CG	4:A:550:DHB:C6	2.92	0.47
2:F:326:THR:O	2:F:326:THR:HG22	2.14	0.47
2:H:429:CME:SD	2:H:429:CME:CZ	3.02	0.47
1:G:133:ARG:HB2	4:H:3550:DHB:O1	2.15	0.47
2:J:376:GLU:HB3	5:J:4665:HOH:O	2.14	0.47
2:J:321:THR:HG21	2:J:494:SER:HB2	1.97	0.47
1:C:131:PHE:O	1:C:132:ALA:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:310:ILE:HD12	2:L:453:PRO:HB2	1.96	0.47
1:G:38:ARG:NH1	1:G:38:ARG:HG3	2.23	0.47
1:K:144:TYR:CZ	1:K:158:LEU:HD22	2.50	0.47
2:L:522:ARG:HD3	2:L:522:ARG:HH11	1.44	0.47
1:C:23:LEU:HD12	1:C:23:LEU:N	2.30	0.46
1:G:25:ALA:HB1	1:G:98:THR:HG21	1.97	0.46
2:J:426:VAL:CG2	2:J:426:VAL:CG1	2.78	0.46
2:D:315:TRP:HZ2	2:D:503:GLN:NE2	2.13	0.46
1:A:70:VAL:HG12	1:A:128:ILE:HG12	1.97	0.46
1:E:184:ARG:HH11	1:E:184:ARG:HG3	1.80	0.46
1:E:184:ARG:HG3	1:E:184:ARG:NH1	2.29	0.46
1:K:131:PHE:CZ	2:L:473:LYS:HE2	2.50	0.46
1:E:92:PHE:CG	2:F:349:PRO:HG3	2.50	0.46
2:H:325:LYS:HE2	5:J:4727:HOH:O	2.15	0.46
2:F:361:HIS:ND1	2:F:429:CME:HZ2	2.31	0.46
2:B:369:ASN:H	2:B:422:ASN:ND2	2.14	0.46
2:D:356:PHE:CZ	2:D:430:LEU:HD13	2.50	0.46
2:F:408:HIS:NE2	5:F:2901:HOH:O	2.23	0.46
1:I:85:LEU:HA	1:I:85:LEU:HD23	1.71	0.46
2:L:437:TYR:OH	2:L:523:PHE:HB3	2.16	0.46
1:K:20:GLY:O	1:K:21:LEU:HD23	2.16	0.46
2:B:356:PHE:CE2	2:B:430:LEU:HD22	2.51	0.46
2:B:484:PRO:O	2:B:487:PRO:HD2	2.16	0.46
1:C:190:GLN:HG3	2:D:333:ARG:HG2	1.97	0.46
1:K:160:LEU:HD23	1:K:160:LEU:HA	1.78	0.46
2:L:315:TRP:HZ2	2:L:503:GLN:NE2	2.13	0.46
1:E:71:TRP:HA	1:E:91:SER:O	2.16	0.46
1:K:190:GLN:HG3	2:L:333:ARG:HG2	1.98	0.46
2:J:307:ARG:HG2	2:J:533:THR:HG22	1.98	0.45
2:B:491:ILE:HG21	2:B:491:ILE:HD13	1.76	0.45
1:C:114:VAL:HG23	1:C:122:MET:CE	2.46	0.45
1:E:143:LEU:HD23	1:E:143:LEU:C	2.37	0.45
2:D:393:PRO:HB3	2:D:433:SER:O	2.16	0.45
1:C:160:LEU:HD23	1:C:160:LEU:HA	1.69	0.45
2:J:495:ILE:HG21	2:J:500:ALA:HB3	1.99	0.45
1:I:58:GLY:HA3	1:I:190:GLN:OE1	2.16	0.45
2:B:364:LEU:HD22	2:B:440:ARG:CD	2.35	0.45
2:L:449:TRP:N	2:L:449:TRP:CD1	2.84	0.45
2:F:343:ILE:HG23	2:F:344:SER:N	2.32	0.45
2:H:405:GLY:HA3	5:H:950:HOH:O	2.16	0.45
2:H:364:LEU:CD1	2:H:442:ILE:HG23	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:53:GLY:HA3	1:K:185:PHE:O	2.17	0.45
1:K:131:PHE:CD2	1:K:138:HIS:HB3	2.52	0.45
1:E:131:PHE:CD2	2:F:475:ILE:HD12	2.52	0.45
1:C:161:ILE:HD13	1:C:196:VAL:HG21	1.99	0.45
1:E:167:ARG:O	1:E:171:ILE:HD12	2.16	0.45
2:D:379:ILE:HG21	2:D:379:ILE:HD13	1.69	0.45
2:L:497:ASN:C	2:L:497:ASN:ND2	2.70	0.44
2:D:363:LEU:N	2:D:363:LEU:HD12	2.31	0.44
2:F:390:LYS:HD3	5:F:2677:HOH:O	2.17	0.44
1:A:163:GLN:CD	1:A:163:GLN:CB	2.75	0.44
1:I:19:ILE:HG22	1:I:26:ALA:HB1	1.98	0.44
1:C:131:PHE:CD2	1:C:138:HIS:HB3	2.53	0.44
1:K:64:ARG:NH1	1:K:99:PHE:O	2.51	0.44
2:J:356:PHE:HZ	2:J:430:LEU:HD13	1.82	0.44
2:L:441:THR:OG1	2:L:442:ILE:N	2.50	0.44
2:F:368:ASN:ND2	2:F:371:GLY:N	2.56	0.44
1:C:26:ALA:O	2:D:411:LYS:NZ	2.42	0.44
1:G:70:VAL:HG21	1:G:106:LEU:HD21	2.00	0.44
2:D:511:ASN:ND2	2:D:511:ASN:H	2.15	0.44
1:G:177:VAL:O	1:G:180:LYS:HB3	2.16	0.43
2:J:361:HIS:N	2:J:361:HIS:CD2	2.72	0.43
1:A:61:HIS:ND1	1:C:163:GLN:HG3	2.33	0.43
2:F:304:ASP:OD1	2:F:307:ARG:NH1	2.40	0.43
1:C:53:GLY:HA3	1:C:185:PHE:O	2.18	0.43
2:H:333:ARG:HD3	2:H:333:ARG:HA	1.74	0.43
2:B:348:GLY:HA3	2:B:469:SER:HA	2.00	0.43
2:J:532:LYS:CB	2:J:532:LYS:HA	2.19	0.43
2:J:363:LEU:N	2:J:363:LEU:HD12	2.34	0.43
2:B:489:CYS:SG	2:B:492:VAL:HG23	2.58	0.43
1:K:35:ILE:HG22	1:K:94:ARG:HG3	2.01	0.43
1:C:26:ALA:C	2:D:411:LYS:HZ2	2.21	0.43
1:G:98:THR:N	1:G:101:ALA:O	2.47	0.43
1:C:155:CYS:O	1:C:159:ASN:ND2	2.51	0.43
2:F:364:LEU:HD22	2:F:440:ARG:HG2	2.00	0.43
1:A:163:GLN:HA	1:A:164:PRO:HD2	1.89	0.43
2:H:497:ASN:ND2	2:H:499:GLU:H	2.14	0.43
1:I:67:PHE:CZ	1:I:94:ARG:HD2	2.54	0.43
1:C:70:VAL:HG12	1:C:128:ILE:HG12	2.00	0.43
1:I:26:ALA:O	2:J:411:LYS:NZ	2.49	0.43
2:J:460:HIS:ND1	2:J:460:HIS:N	2.67	0.43
1:I:115:ASN:HA	1:I:121:PRO:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:PRO:HD3	4:A:550:DHB:C2	2.48	0.43
2:J:338:SER:HB2	5:J:3694:HOH:O	2.18	0.43
1:I:133:ARG:HB2	4:J:4550:DHB:O1	2.19	0.43
1:A:160:LEU:HA	1:A:160:LEU:HD23	1.75	0.43
2:B:400:TRP:HA	2:B:425:GLY:O	2.18	0.43
2:J:386:ASP:HB2	2:J:529:GLY:HA2	2.00	0.42
1:C:48:HIS:N	1:C:48:HIS:CD2	2.86	0.42
2:H:460:HIS:N	2:H:460:HIS:ND1	2.67	0.42
1:A:64:ARG:NH1	1:A:99:PHE:O	2.51	0.42
1:G:113:VAL:HG22	1:G:124:PRO:HD3	2.00	0.42
1:A:155:CYS:HB3	1:A:158:LEU:HB2	2.01	0.42
2:J:361:HIS:H	2:J:361:HIS:HD2	1.58	0.42
2:D:376:GLU:HG3	2:D:376:GLU:H	1.67	0.42
2:B:318:LYS:CD	2:B:318:LYS:NZ	2.73	0.42
1:E:92:PHE:CD1	2:F:349:PRO:HG3	2.53	0.42
2:J:356:PHE:CZ	2:J:430:LEU:HD13	2.54	0.42
2:J:364:LEU:HD22	2:J:440:ARG:HG2	2.01	0.42
2:B:333:ARG:HD3	2:B:333:ARG:HA	1.81	0.42
2:J:442:ILE:H	2:J:442:ILE:HG13	1.72	0.42
1:E:131:PHE:CE2	1:E:138:HIS:HB3	2.55	0.42
1:A:4:LEU:HA	1:A:4:LEU:HD12	1.83	0.42
2:H:308:PHE:O	2:H:309:VAL:C	2.56	0.42
1:G:31:ARG:HH12	2:H:428:ARG:HG2	1.84	0.42
2:F:437:TYR:OH	2:F:523:PHE:HB3	2.20	0.42
2:H:379:ILE:HG21	2:H:379:ILE:HD13	1.79	0.42
2:L:314:ASN:OD1	2:L:318:LYS:HE2	2.20	0.42
1:K:51:LEU:HA	1:K:51:LEU:HD23	1.91	0.42
2:J:489:CYS:HA	2:J:490:PRO:HD3	1.84	0.42
1:A:165:GLN:N	1:A:165:GLN:NE2	2.44	0.42
1:I:160:LEU:HD23	1:I:160:LEU:HA	1.79	0.42
1:I:157:VAL:O	1:I:160:LEU:HB2	2.20	0.42
1:G:67:PHE:CE1	1:G:94:ARG:HD2	2.53	0.41
2:J:325:LYS:HG2	2:L:335:ALA:HB1	2.02	0.41
2:L:447:TYR:HA	2:L:448:PRO:HD3	1.94	0.41
1:G:15:PRO:CD	4:H:3550:DHB:C2	2.98	0.41
1:K:72:GLN:O	1:K:72:GLN:HG3	2.19	0.41
2:F:411:LYS:CG	2:F:411:LYS:CE	2.86	0.41
1:C:98:THR:O	1:C:101:ALA:O	2.38	0.41
2:F:372:LEU:HA	2:F:373:PRO:HD3	1.84	0.41
1:E:26:ALA:O	2:F:411:LYS:NZ	2.46	0.41
1:A:15:PRO:HG2	4:A:550:DHB:C6	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:GLN:HG3	2:B:333:ARG:HG2	2.01	0.41
1:K:71:TRP:HZ2	2:L:347:THR:HG1	1.64	0.41
1:G:52:LEU:CD2	1:G:184:ARG:NH1	2.83	0.41
2:J:478:LEU:C	2:J:478:LEU:HD23	2.41	0.41
2:J:461:ILE:HG22	2:J:462:HIS:O	2.20	0.41
1:K:125:HIS:HA	1:K:143:LEU:O	2.20	0.41
2:B:446:PRO:HD2	2:H:376:GLU:HG2	2.02	0.41
1:A:85:LEU:HD23	1:A:85:LEU:HA	1.69	0.41
2:H:335:ALA:HB1	2:L:325:LYS:HG2	2.02	0.41
1:I:131:PHE:CD2	1:I:138:HIS:HB3	2.55	0.41
2:H:495:ILE:CG2	2:H:500:ALA:HB3	2.50	0.41
1:A:71:TRP:CZ3	1:A:91:SER:HB3	2.54	0.41
1:C:138:HIS:ND1	1:C:138:HIS:N	2.68	0.41
1:C:143:LEU:C	1:C:143:LEU:HD23	2.41	0.41
2:L:437:TYR:HH	2:L:523:PHE:HB3	1.85	0.41
1:C:200:PHE:HB3	2:D:339:ILE:HG13	2.02	0.41
1:G:189:ILE:HD13	1:G:189:ILE:HG21	1.82	0.41
2:H:386:ASP:C	2:H:386:ASP:OD2	2.59	0.41
1:K:50:LEU:O	1:K:182:ALA:HA	2.21	0.41
2:F:411:LYS:NZ	2:F:411:LYS:H	2.12	0.41
2:B:390:LYS:CG	2:B:390:LYS:CE	2.87	0.41
2:H:486:ILE:O	2:H:488:MET:N	2.54	0.41
2:F:437:TYR:O	2:F:438:SER:HB3	2.21	0.41
2:F:399:MET:HA	2:F:462:HIS:O	2.21	0.41
2:H:522:ARG:HH11	2:H:522:ARG:HD3	1.67	0.41
1:A:50:LEU:O	1:A:182:ALA:HA	2.20	0.41
2:D:314:ASN:OD1	2:D:318:LYS:HE2	2.21	0.41
1:E:2:ILE:HD13	1:E:2:ILE:HA	1.84	0.41
2:F:411:LYS:O	2:F:414:ARG:NH1	2.40	0.41
1:I:15:PRO:HD3	4:J:4550:DHB:C1	2.51	0.41
2:L:478:LEU:HD12	2:L:523:PHE:CD2	2.56	0.41
2:F:485:LEU:HA	2:F:485:LEU:HD23	1.91	0.41
2:H:400:TRP:HA	2:H:425:GLY:O	2.21	0.41
2:J:454:ASN:HB2	2:L:310:ILE:HG13	2.03	0.40
2:B:517:ASP:C	2:B:517:ASP:OD1	2.59	0.40
2:D:381:ALA:O	2:D:522:ARG:HA	2.21	0.40
1:K:92:PHE:CG	2:L:349:PRO:HG3	2.57	0.40
2:B:368:ASN:HD22	2:B:371:GLY:H	1.70	0.40
2:L:451:ASN:HB3	2:L:455:ASP:OD2	2.20	0.40
2:L:516:MET:CE	2:L:516:MET:HB3	2.51	0.40
2:D:411:LYS:NZ	2:D:411:LYS:H	2.18	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:360:ASP:OD2	2:H:428:ARG:HD2	2.21	0.40
1:K:92:PHE:CD1	2:L:349:PRO:HG3	2.56	0.40
2:J:420:ASP:HA	2:J:421:PRO:HD2	1.86	0.40
2:L:311:ARG:HD2	2:L:311:ARG:HH11	1.65	0.40
1:K:26:ALA:O	2:L:411:LYS:NZ	2.51	0.40
2:D:408:HIS:HE1	2:D:447:TYR:CZ	2.38	0.40
1:A:80:GLN:O	1:A:91:SER:HB2	2.20	0.40
2:F:483:ASP:HB3	2:F:486:ILE:HG13	2.04	0.40
1:G:51:LEU:HD23	1:G:51:LEU:HA	1.74	0.40
1:G:163:GLN:HA	1:G:164:PRO:HD2	1.95	0.40

All (1) 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)
1:G:150:GLN:CD	5:E:2951:HOH:O[3_445]	2.18	0.02

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	198/200 (99%)	186 (94%)	11 (6%)	1 (0%)	34 47
1	C	198/200 (99%)	190 (96%)	8 (4%)	0	100 100
1	E	198/200 (99%)	189 (96%)	9 (4%)	0	100 100
1	G	198/200 (99%)	189 (96%)	9 (4%)	0	100 100
1	I	198/200 (99%)	187 (94%)	10 (5%)	1 (0%)	34 47
1	K	198/200 (99%)	189 (96%)	7 (4%)	2 (1%)	19 27
2	B	235/238 (99%)	223 (95%)	10 (4%)	2 (1%)	21 29
2	D	235/238 (99%)	225 (96%)	9 (4%)	1 (0%)	39 54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	235/238 (99%)	226 (96%)	8 (3%)	1 (0%)	39	54
2	H	235/238 (99%)	223 (95%)	11 (5%)	1 (0%)	39	54
2	J	235/238 (99%)	222 (94%)	12 (5%)	1 (0%)	39	54
2	L	235/238 (99%)	218 (93%)	15 (6%)	2 (1%)	21	29
All	All	2598/2628 (99%)	2467 (95%)	119 (5%)	12 (0%)	34	47

All (12) 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	B	493	LYS
2	L	493	LYS
1	A	74	ASP
1	I	132	ALA
1	K	179	GLY
1	K	42	PRO

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%)	151 (93%)	11 (7%)	20	30
1	C	162/163 (99%)	149 (92%)	13 (8%)	15	22
1	E	162/163 (99%)	152 (94%)	10 (6%)	23	35
1	G	162/163 (99%)	151 (93%)	11 (7%)	20	30
1	I	162/163 (99%)	151 (93%)	11 (7%)	20	30
1	K	162/163 (99%)	149 (92%)	13 (8%)	15	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	199/201 (99%)	184 (92%)	15 (8%)	17 26
2	D	199/201 (99%)	179 (90%)	20 (10%)	9 13
2	F	199/201 (99%)	181 (91%)	18 (9%)	12 17
2	H	199/201 (99%)	180 (90%)	19 (10%)	11 15
2	J	199/201 (99%)	177 (89%)	22 (11%)	8 10
2	L	199/201 (99%)	179 (90%)	20 (10%)	9 13
All	All	2166/2184 (99%)	1983 (92%)	183 (8%)	14 20

All (183) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	19	ILE
1	A	52	LEU
1	A	91	SER
1	A	114	VAL
1	A	137	ILE
1	A	154	LYS
1	A	158	LEU
1	A	165	GLN
1	A	188	ARG
1	A	192	GLU
2	B	364	LEU
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	468	PRO
2	B	497	ASN
2	B	507	LYS
2	B	512	ASN
2	B	534	HIS
1	C	4	LEU
1	C	6	PRO
1	C	19	ILE

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Mol	Chain	Res	Type
1	C	52	LEU
1	C	76	ASN
1	C	124	PRO
1	C	133	ARG
1	C	154	LYS
1	C	158	LEU
1	C	164	PRO
1	C	165	GLN
1	C	180	LYS
1	C	188	ARG
2	D	364	LEU
2	D	368	ASN
2	D	372	LEU
2	D	390	LYS
2	D	393	PRO
2	D	395	THR
2	D	411	LYS
2	D	414	ARG
2	D	416	LEU
2	D	428	ARG
2	D	433	SER
2	D	442	ILE
2	D	457	ARG
2	D	468	PRO
2	D	473	LYS
2	D	497	ASN
2	D	512	ASN
2	D	533	THR
2	D	534	HIS
2	D	538	CYS
1	E	4	LEU
1	E	19	ILE
1	E	52	LEU
1	E	66	SER
1	E	98	THR
1	E	114	VAL
1	E	158	LEU
1	E	165	GLN
1	E	180	LYS
1	E	192	GLU
2	F	364	LEU
2	F	372	LEU

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Mol	Chain	Res	Type
2	F	393	PRO
2	F	395	THR
2	F	411	LYS
2	F	416	LEU
2	F	428	ARG
2	F	433	SER
2	F	434	ASP
2	F	442	ILE
2	F	449	TRP
2	F	457	ARG
2	F	478	LEU
2	F	497	ASN
2	F	503	GLN
2	F	515	PRO
2	F	522	ARG
2	F	534	HIS
1	G	4	LEU
1	G	19	ILE
1	G	36	TRP
1	G	38	ARG
1	G	52	LEU
1	G	66	SER
1	G	91	SER
1	G	98	THR
1	G	133	ARG
1	G	158	LEU
1	G	165	GLN
2	H	364	LEU
2	H	368	ASN
2	H	372	LEU
2	H	390	LYS
2	H	391	PRO
2	H	395	THR
2	H	399	MET
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	466	SER
2	H	473	LYS

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Mol	Chain	Res	Type
2	H	497	ASN
2	H	507	LYS
2	H	511	ASN
2	H	534	HIS
1	I	4	LEU
1	I	19	ILE
1	I	38	ARG
1	I	42	PRO
1	I	52	LEU
1	I	94	ARG
1	I	133	ARG
1	I	165	GLN
1	I	168	GLU
1	I	180	LYS
1	I	192	GLU
2	J	338	SER
2	J	364	LEU
2	J	372	LEU
2	J	390	LYS
2	J	395	THR
2	J	399	MET
2	J	411	LYS
2	J	414	ARG
2	J	416	LEU
2	J	428	ARG
2	J	433	SER
2	J	434	ASP
2	J	442	ILE
2	J	457	ARG
2	J	473	LYS
2	J	478	LEU
2	J	497	ASN
2	J	503	GLN
2	J	507	LYS
2	J	512	ASN
2	J	534	HIS
2	J	538	CYS
1	K	4	LEU
1	K	19	ILE
1	K	42	PRO
1	K	52	LEU
1	K	66	SER

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Mol	Chain	Res	Type
1	K	76	ASN
1	K	94	ARG
1	K	106	LEU
1	K	114	VAL
1	K	122	MET
1	K	133	ARG
1	K	158	LEU
1	K	165	GLN
2	L	306	SER
2	L	364	LEU
2	L	372	LEU
2	L	390	LYS
2	L	393	PRO
2	L	394	ASN
2	L	395	THR
2	L	411	LYS
2	L	414	ARG
2	L	416	LEU
2	L	428	ARG
2	L	433	SER
2	L	449	TRP
2	L	457	ARG
2	L	478	LEU
2	L	497	ASN
2	L	507	LYS
2	L	534	HIS
2	L	537	ASN
2	L	538	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	GLN
2	B	361	HIS
2	B	368	ASN
2	B	369	ASN
2	B	412	ASN
2	B	422	ASN
2	B	497	ASN
2	B	503	GLN
1	C	165	GLN
2	D	361	HIS

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Mol	Chain	Res	Type
2	D	368	ASN
2	D	369	ASN
2	D	412	ASN
2	D	422	ASN
2	D	497	ASN
2	D	503	GLN
1	E	107	HIS
1	E	165	GLN
2	F	361	HIS
2	F	368	ASN
2	F	369	ASN
2	F	422	ASN
2	F	497	ASN
2	F	503	GLN
1	G	163	GLN
1	G	165	GLN
2	H	361	HIS
2	H	368	ASN
2	H	412	ASN
2	H	422	ASN
2	H	497	ASN
2	H	503	GLN
1	I	165	GLN
2	J	361	HIS
2	J	368	ASN
2	J	369	ASN
2	J	412	ASN
2	J	422	ASN
2	J	497	ASN
2	J	503	GLN
1	K	165	GLN
2	L	361	HIS
2	L	368	ASN
2	L	369	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 (i)

6 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	CME	B	429	2	8,9,10	1.87	3 (37%)	6,9,11	3.64	3 (50%)
2	CME	D	429	2	8,9,10	2.23	3 (37%)	6,9,11	2.17	4 (66%)
2	CME	F	429	2	8,9,10	3.24	3 (37%)	6,9,11	2.20	3 (50%)
2	CME	H	429	2	8,9,10	2.73	5 (62%)	6,9,11	1.92	2 (33%)
2	CME	J	429	2	8,9,10	1.85	3 (37%)	6,9,11	2.10	3 (50%)
2	CME	L	429	2	8,9,10	2.01	2 (25%)	6,9,11	2.97	5 (83%)

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
2	CME	B	429	2	-	0/5/8/10	0/0/0/0
2	CME	D	429	2	-	0/5/8/10	0/0/0/0
2	CME	F	429	2	-	0/5/8/10	0/0/0/0
2	CME	H	429	2	-	0/5/8/10	0/0/0/0
2	CME	J	429	2	-	0/5/8/10	0/0/0/0
2	CME	L	429	2	-	0/5/8/10	0/0/0/0

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	429	CME	CB-SG	-7.28	1.56	1.81
2	D	429	CME	CB-SG	-4.92	1.64	1.81
2	H	429	CME	CB-SG	-4.45	1.65	1.81
2	B	429	CME	CB-SG	-3.52	1.69	1.81
2	F	429	CME	CB-CA	-3.43	1.44	1.53
2	J	429	CME	CB-SG	-3.34	1.69	1.81
2	F	429	CME	CA-N	-3.34	1.37	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	429	CME	CB-SG	-2.85	1.71	1.81
2	D	429	CME	CA-N	-2.39	1.40	1.47
2	D	429	CME	CB-CA	-2.11	1.47	1.53
2	J	429	CME	CB-CA	-2.05	1.47	1.53
2	H	429	CME	CB-CA	-2.02	1.47	1.53
2	J	429	CME	CE-CZ	2.09	1.65	1.49
2	B	429	CME	CE-CZ	2.13	1.65	1.49
2	B	429	CME	CE-SD	2.26	1.93	1.82
2	H	429	CME	O-C	2.43	1.31	1.19
2	H	429	CME	CE-SD	3.33	1.98	1.82
2	L	429	CME	CE-CZ	3.70	1.77	1.49
2	H	429	CME	CE-CZ	3.97	1.79	1.49

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	429	CME	CZ-CE-SD	-4.63	101.84	113.16
2	L	429	CME	CB-SG-SD	-3.40	97.33	103.95
2	B	429	CME	O-C-CA	-3.11	117.38	125.49
2	H	429	CME	CZ-CE-SD	-2.83	106.25	113.16
2	J	429	CME	CZ-CE-SD	-2.72	106.51	113.16
2	F	429	CME	CZ-CE-SD	-2.71	106.54	113.16
2	L	429	CME	O-C-CA	-2.51	118.95	125.49
2	J	429	CME	CB-SG-SD	-2.28	99.51	103.95
2	D	429	CME	O-C-CA	-2.28	119.56	125.49
2	D	429	CME	CB-SG-SD	-2.19	99.68	103.95
2	F	429	CME	OH-CZ-CE	2.19	120.42	110.83
2	L	429	CME	OH-CZ-CE	2.40	121.35	110.83
2	H	429	CME	OH-CZ-CE	2.51	121.81	110.83
2	B	429	CME	OH-CZ-CE	2.53	121.92	110.83
2	L	429	CME	CE-SD-SG	2.58	116.95	103.56
2	D	429	CME	CE-SD-SG	2.70	117.56	103.56
2	J	429	CME	OH-CZ-CE	2.83	123.22	110.83
2	D	429	CME	OH-CZ-CE	3.18	124.75	110.83
2	F	429	CME	CE-SD-SG	3.57	122.06	103.56
2	B	429	CME	CB-SG-SD	7.60	118.76	103.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	429	CME	1	0
2	H	429	CME	2	0
2	L	429	CME	2	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

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	A	550	3,2	8,11,11	0.88	0	11,15,15	0.87	0
4	DHB	D	1550	3	8,11,11	0.93	0	11,15,15	0.57	0
4	DHB	F	2550	3	8,11,11	1.15	0	11,15,15	0.65	0
4	DHB	H	3550	3	8,11,11	0.92	0	11,15,15	0.60	0
4	DHB	J	4550	3	8,11,11	0.75	0	11,15,15	0.69	0
4	DHB	L	5550	3,2	8,11,11	0.77	0	11,15,15	0.69	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	A	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	3	-	0/0/4/4	0/1/1/1
4	DHB	L	5550	3,2	-	0/0/4/4	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

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	A	550	DHB	6	0
4	D	1550	DHB	1	0
4	F	2550	DHB	1	0
4	H	3550	DHB	6	0
4	J	4550	DHB	3	0
4	L	5550	DHB	3	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%)	-0.71	2 (1%)	84 83	9, 24, 57, 73	0
1	C	200/200 (100%)	-0.67	3 (1%)	76 75	8, 25, 57, 72	0
1	E	200/200 (100%)	-0.60	2 (1%)	84 83	7, 27, 57, 73	0
1	G	200/200 (100%)	-0.61	4 (2%)	68 67	8, 26, 58, 73	0
1	I	200/200 (100%)	-0.51	4 (2%)	68 67	9, 28, 59, 73	0
1	K	200/200 (100%)	-0.27	10 (5%)	32 32	12, 30, 59, 73	0
2	B	237/238 (99%)	-0.84	3 (1%)	79 79	9, 19, 48, 68	0
2	D	237/238 (99%)	-0.83	4 (1%)	73 72	8, 19, 48, 68	0
2	F	237/238 (99%)	-0.88	3 (1%)	79 79	8, 19, 48, 67	0
2	H	237/238 (99%)	-0.92	2 (0%)	87 87	9, 19, 48, 65	0
2	J	237/238 (99%)	-0.87	3 (1%)	79 79	11, 22, 49, 68	0
2	L	237/238 (99%)	-0.77	5 (2%)	67 66	12, 21, 50, 68	0
All	All	2622/2628 (99%)	-0.72	45 (1%)	73 72	7, 23, 56, 73	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	99	PHE	4.6
2	L	301	PRO	4.2
1	G	100	ASP	4.0
1	I	98	THR	3.8
2	F	368	ASN	3.8
1	I	100	ASP	3.7
2	L	368	ASN	3.6
1	E	99	PHE	3.6
2	L	370	GLY	3.6
1	A	99	PHE	3.5
1	E	100	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
1	K	179	GLY	3.5
2	B	368	ASN	3.3
2	D	301	PRO	3.3
1	K	99	PHE	3.3
1	K	177	VAL	3.2
1	I	99	PHE	3.2
1	K	178	ASP	3.1
2	F	370	GLY	3.1
1	K	101	ALA	3.1
2	D	368	ASN	3.0
2	D	538	CYS	3.0
1	I	177	VAL	2.9
2	H	537	ASN	2.7
1	K	100	ASP	2.6
1	C	98	THR	2.5
1	G	177	VAL	2.4
1	C	100	ASP	2.3
1	C	99	PHE	2.3
2	J	368	ASN	2.3
2	B	370	GLY	2.2
2	D	411	LYS	2.2
2	J	370	GLY	2.2
2	J	537	ASN	2.2
1	G	27	GLY	2.1
1	K	119	GLY	2.1
2	H	301	PRO	2.1
1	K	86	GLU	2.1
2	L	414	ARG	2.0
2	F	301	PRO	2.0
1	K	150	GLN	2.0
1	A	100	ASP	2.0
1	K	43	ASP	2.0
2	B	369	ASN	2.0
2	L	537	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
2	CME	H	429	10/11	0.97	0.09	-	23,31,52,52	0
2	CME	B	429	10/11	0.97	0.10	-	22,30,52,55	0
2	CME	D	429	10/11	0.97	0.11	-	23,32,55,57	0
2	CME	J	429	10/11	0.96	0.09	-	26,33,55,57	0
2	CME	L	429	10/11	0.96	0.13	-	25,34,55,57	0
2	CME	F	429	10/11	0.96	0.10	-	23,31,53,56	0

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	J	4550	11/11	0.88	0.31	15.06	103,105,106,106	0
4	DHB	H	3550	11/11	0.83	0.28	14.66	100,101,101,102	0
4	DHB	F	2550	11/11	0.83	0.34	13.07	102,102,103,103	0
4	DHB	L	5550	11/11	0.85	0.26	10.91	86,87,88,88	0
4	DHB	A	550	11/11	0.85	0.28	10.06	86,88,88,89	0
4	DHB	D	1550	11/11	0.87	0.23	7.17	77,78,79,79	0
3	FE	F	2600	1/1	0.99	0.09	0.14	57,57,57,57	0
3	FE	J	4600	1/1	0.90	0.07	-0.74	67,67,67,67	0
3	FE	B	600	1/1	0.94	0.08	-1.00	62,62,62,62	0
3	FE	L	5600	1/1	0.92	0.06	-1.52	63,63,63,63	0
3	FE	D	1600	1/1	0.98	0.06	-1.62	54,54,54,54	0
3	FE	H	3600	1/1	0.92	0.04	-3.07	63,63,63,63	0

6.5 Other polymers (i)

There are no such residues in this entry.