Full wwPDB X-ray Structure Validation Report (i)

Oct 12, 2021 – 11:26 AM EDT

PDB ID	:	1YKN
Title	:	Protocatechuate 3,4-dioxygenase Y408E mutant bound to DHB
Authors	:	Brown, C.K.; Ohlendorf, D.H.
Deposited on	:	2005-01-18
Resolution	:	2.06 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

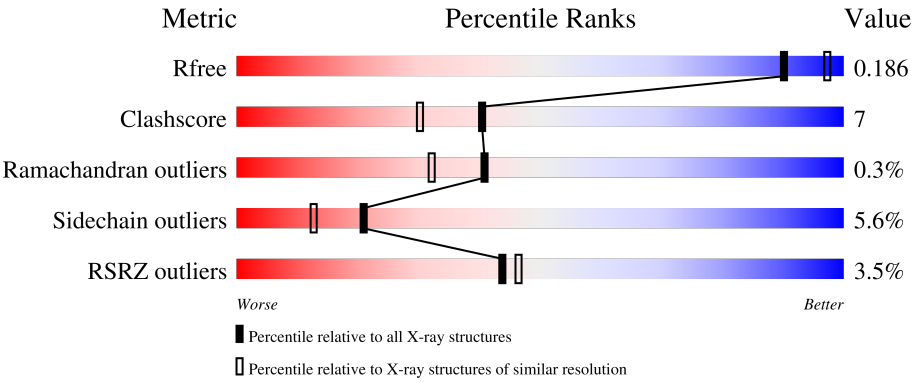
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.06 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2684 (2.08-2.04)
Clashscore	141614	2801 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)
RSRZ outliers	127900	2646 (2.08-2.04)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	3% 64% 28% 6% •
1	C	200	2% 65% 26% 7% •
1	E	200	4% 58% 36% 6%
1	G	200	4% 62% 28% 8% •
1	I	200	6% 62% 32% 5% •

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Mol	Chain	Length	Quality of chain
1	K	200	6% 66% 28%
2	B	238	3% 61% 28% 10%
2	D	238	3% 66% 27% 6%
2	F	238	3% 60% 32% 6%
2	H	238	3% 62% 31% 7%
2	J	238	3% 60% 32% 7%
2	L	238	3% 60% 33% 6%

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
2	CME	H	429	-	X	-	-
4	DHB	B	550	-	-	X	-
4	DHB	F	2550	-	-	X	-
4	DHB	H	3550	-	-	X	-
4	DHB	L	5550	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 22266 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
			1876	1186	342	339	9			
2	D	238	Total	C	N	O	S	0	0	0
			1876	1186	342	339	9			
2	F	238	Total	C	N	O	S	0	0	0
			1876	1186	342	339	9			
2	H	238	Total	C	N	O	S	0	0	0
			1876	1186	342	339	9			
2	J	238	Total	C	N	O	S	0	0	0
			1876	1186	342	339	9			
2	L	238	Total	C	N	O	S	0	0	0
			1876	1186	342	339	9			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	408	GLU	TYR	engineered mutation	UNP P00437

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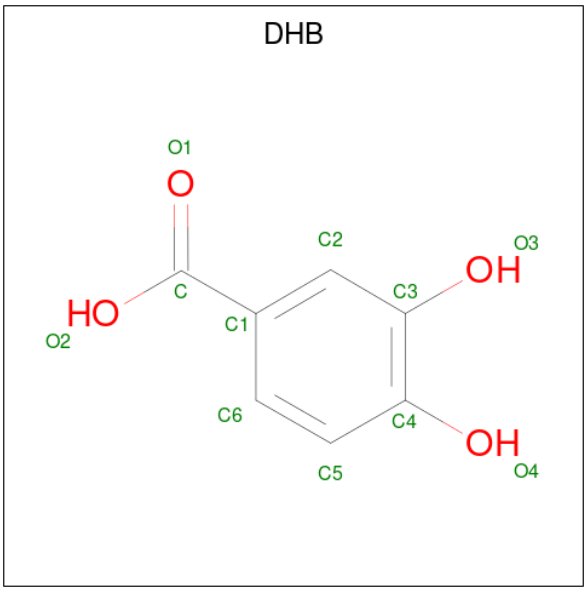
Chain	Residue	Modelled	Actual	Comment	Reference
B	429	CME	CYS	modified residue	UNP P00437
D	408	GLU	TYR	engineered mutation	UNP P00437
D	429	CME	CYS	modified residue	UNP P00437
F	408	GLU	TYR	engineered mutation	UNP P00437
F	429	CME	CYS	modified residue	UNP P00437
H	408	GLU	TYR	engineered mutation	UNP P00437
H	429	CME	CYS	modified residue	UNP P00437
J	408	GLU	TYR	engineered mutation	UNP P00437
J	429	CME	CYS	modified residue	UNP P00437
L	408	GLU	TYR	engineered mutation	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	B	1	Total Fe 1 1	0	0
3	D	1	Total Fe 1 1	0	0
3	F	1	Total Fe 1 1	0	0
3	H	1	Total Fe 1 1	0	0
3	J	1	Total Fe 1 1	0	0
3	L	1	Total Fe 1 1	0	0

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



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	88	Total O 88 88	0	0
5	B	162	Total O 162 162	0	0
5	C	88	Total O 88 88	0	0
5	D	168	Total O 168 168	0	0
5	E	86	Total O 86 86	0	0
5	F	163	Total O 163 163	0	0

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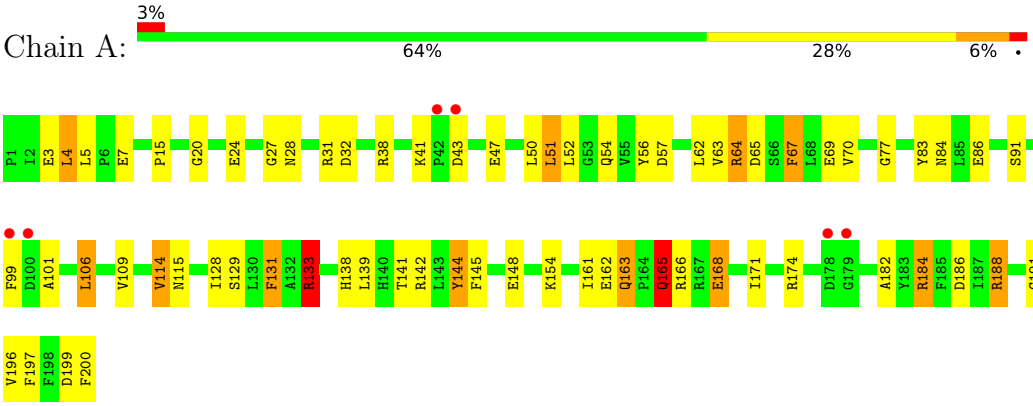
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	G	92	Total O 92 92	0	0
5	H	157	Total O 157 157	0	0
5	I	87	Total O 87 87	0	0
5	J	172	Total O 172 172	0	0
5	K	81	Total O 81 81	0	0
5	L	168	Total O 168 168	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

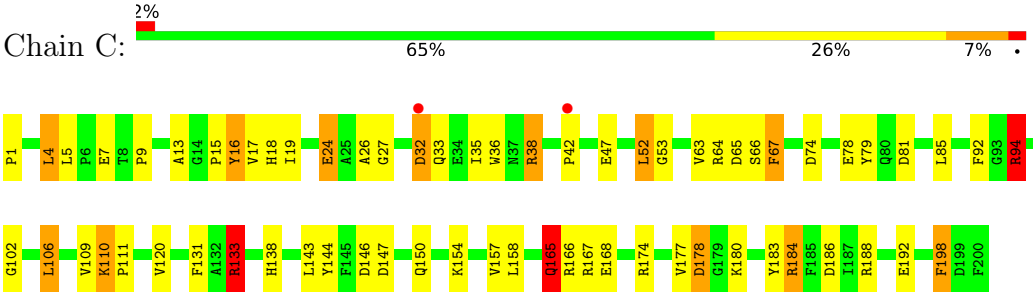
• Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain

Chain A:



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

Chain C:



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

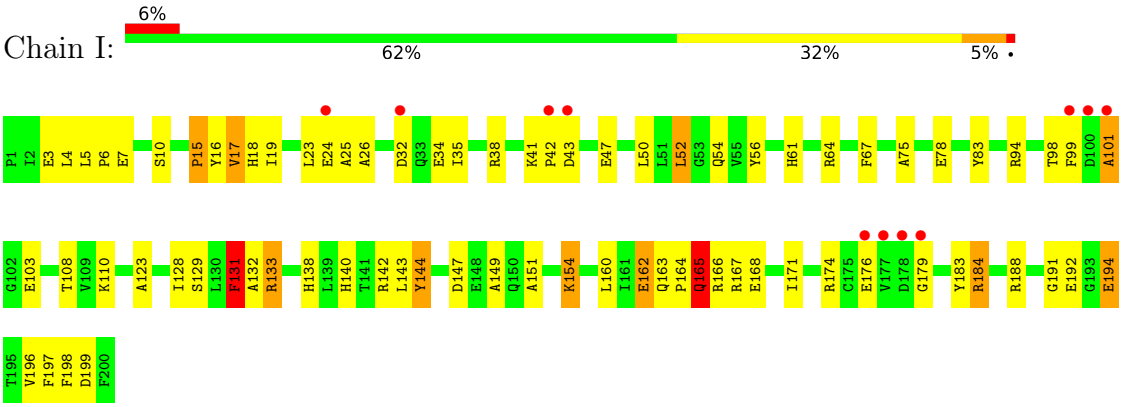
Chain E:

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

Chain G:

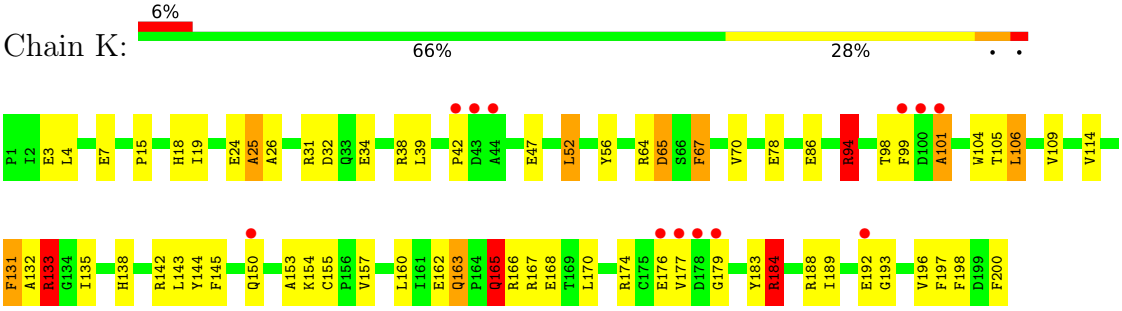
• Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain

Chain I:



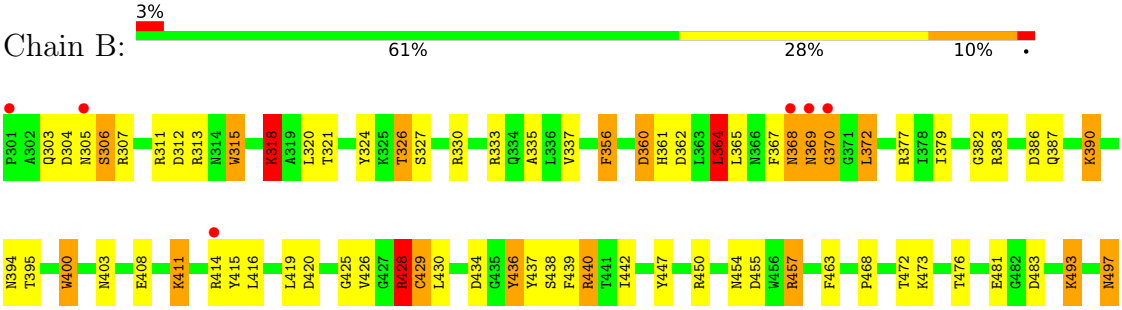
• Molecule 1: Protocatechuate 3,4-dioxygenase alpha chain

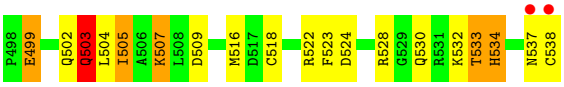
Chain K:



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

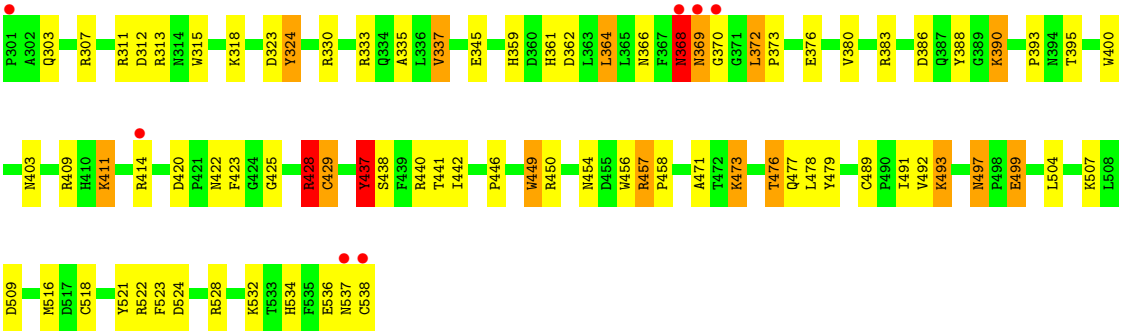
Chain B:





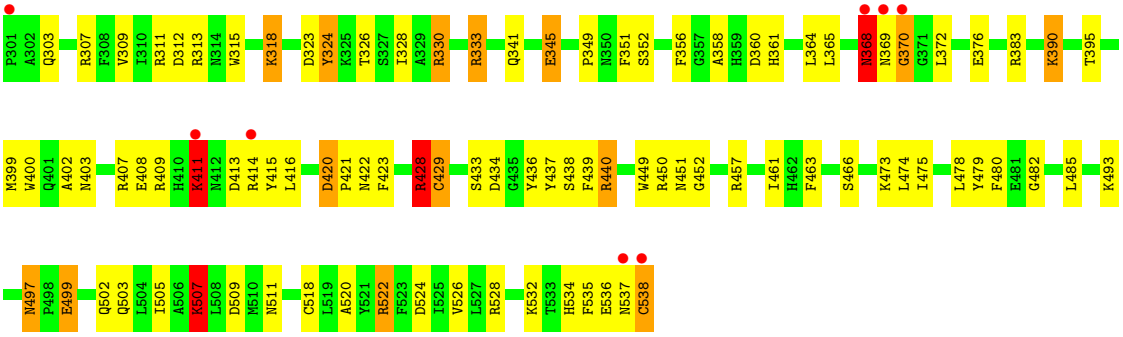
• Molecule 2: Protocatechuate 3,4-dioxygenase beta chain

Chain D:



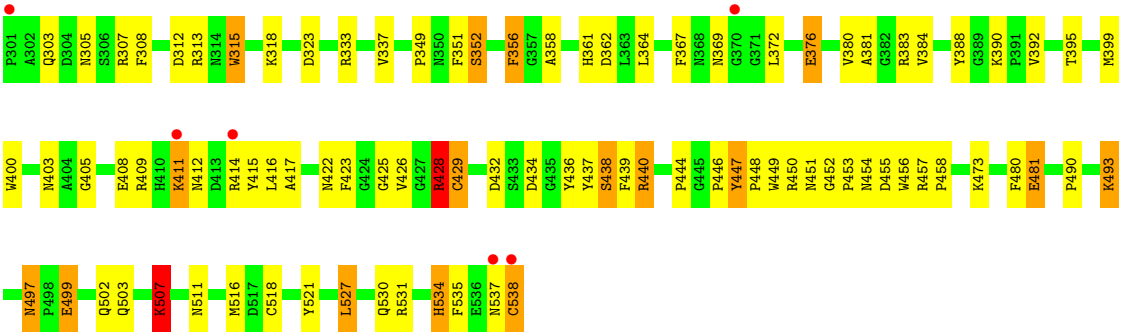
• Molecule 2: Protocatechuate 3,4-dioxygenase beta chain

Chain F:



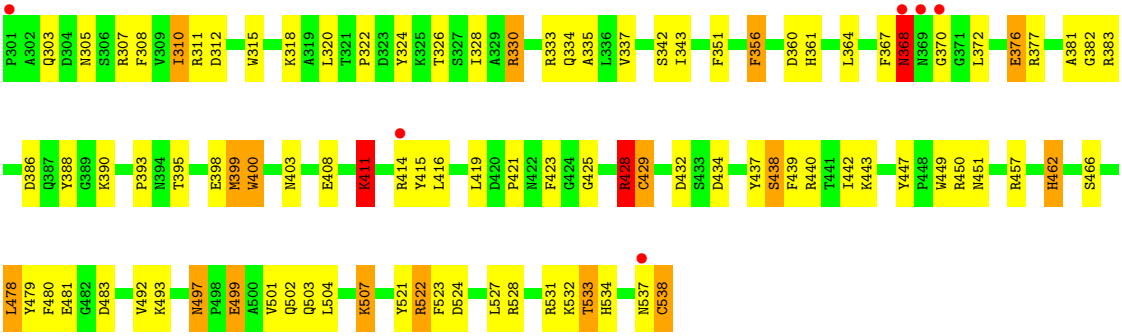
• Molecule 2: Protocatechuate 3,4-dioxygenase beta chain

Chain H:



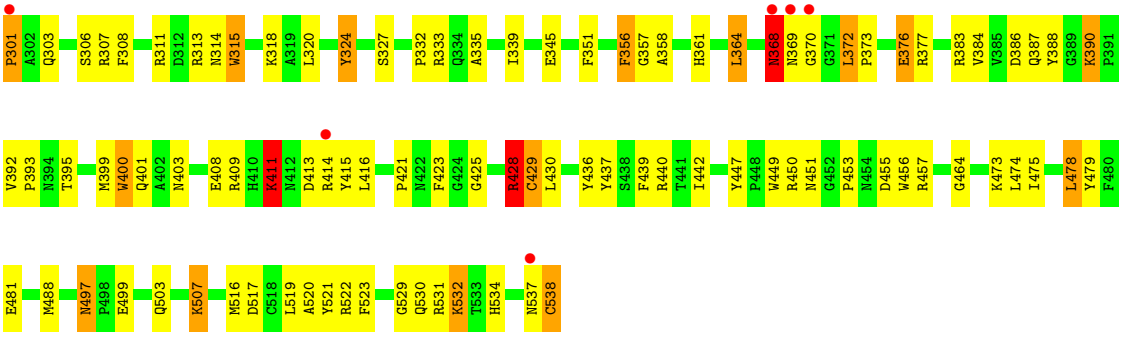
• Molecule 2: Protocatechuate 3,4-dioxygenase beta chain

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	195.82Å 128.57Å 134.36Å 90.00° 97.98° 90.00°	Depositor
Resolution (Å)	8.51 – 2.06 20.06 – 1.94	Depositor EDS
% Data completeness (in resolution range)	69.6 (8.51-2.06) 68.8 (20.06-1.94)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.00 (at 1.94Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.149 , 0.192 0.145 , 0.186	Depositor DCC
R_{free} test set	1950 reflections (0.96%)	wwPDB-VP
Wilson B-factor (Å^2)	16.3	Xtriage
Anisotropy	0.221	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.46 , 66.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	22266	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: FE, DHB, CME

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	2.25	50/1611 (3.1%)	1.68	30/2195 (1.4%)
1	C	2.25	61/1611 (3.8%)	1.90	39/2195 (1.8%)
1	E	2.26	70/1611 (4.3%)	1.56	19/2195 (0.9%)
1	G	2.20	60/1611 (3.7%)	1.74	31/2195 (1.4%)
1	I	2.24	59/1611 (3.7%)	1.71	23/2195 (1.0%)
1	K	2.23	61/1611 (3.8%)	1.72	20/2195 (0.9%)
2	B	2.07	56/1920 (2.9%)	1.81	48/2612 (1.8%)
2	D	2.11	58/1920 (3.0%)	1.75	36/2612 (1.4%)
2	F	2.16	62/1920 (3.2%)	1.91	44/2612 (1.7%)
2	H	2.12	61/1920 (3.2%)	1.75	37/2612 (1.4%)
2	J	2.15	61/1920 (3.2%)	1.76	41/2612 (1.6%)
2	L	2.13	66/1920 (3.4%)	1.79	33/2612 (1.3%)
All	All	2.18	725/21186 (3.4%)	1.76	401/28842 (1.4%)

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	4
1	E	0	5
1	G	0	5
1	I	0	6
1	K	0	3
2	B	0	5
2	D	0	3
2	F	0	4
2	H	0	5
2	J	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	L	0	5
All	All	0	52

All (725) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	168	GLU	CD-OE1	15.12	1.42	1.25
1	A	192	GLU	CG-CD	14.26	1.73	1.51
2	L	532	LYS	CA-CB	13.83	1.84	1.53
2	D	449	TRP	CG-CD1	13.78	1.56	1.36
1	E	168	GLU	CD-OE1	12.07	1.39	1.25
1	E	176	GLU	CD-OE2	11.57	1.38	1.25
1	A	47	GLU	CG-CD	11.42	1.69	1.51
1	K	47	GLU	CD-OE1	11.38	1.38	1.25
2	H	507	LYS	CE-NZ	11.37	1.77	1.49
2	J	388	TYR	CE1-CZ	11.12	1.53	1.38
1	A	192	GLU	CB-CG	11.09	1.73	1.52
1	A	47	GLU	CD-OE1	11.03	1.37	1.25
1	K	144	TYR	CD2-CE2	10.90	1.55	1.39
2	H	315	TRP	CB-CG	-10.71	1.30	1.50
1	G	154	LYS	CD-CE	10.65	1.77	1.51
1	I	168	GLU	CB-CG	10.61	1.72	1.52
2	L	538	CYS	CB-SG	-10.57	1.64	1.82
2	F	324	TYR	CE2-CZ	10.51	1.52	1.38
1	A	168	GLU	CD-OE1	10.43	1.37	1.25
2	B	318	LYS	CE-NZ	10.38	1.75	1.49
1	A	7	GLU	CB-CG	10.18	1.71	1.52
1	E	192	GLU	CG-CD	10.18	1.67	1.51
2	F	415	TYR	CD1-CE1	-10.12	1.24	1.39
1	A	47	GLU	CD-OE2	10.08	1.36	1.25
1	C	192	GLU	CG-CD	9.97	1.67	1.51
1	E	192	GLU	CD-OE1	9.97	1.36	1.25
1	C	192	GLU	CD-OE2	9.92	1.36	1.25
1	C	24	GLU	CG-CD	9.89	1.66	1.51
2	D	376	GLU	CD-OE1	9.83	1.36	1.25
2	F	449	TRP	CG-CD1	9.83	1.50	1.36
1	G	47	GLU	CD-OE2	9.67	1.36	1.25
1	E	47	GLU	CD-OE1	9.55	1.36	1.25
1	K	47	GLU	CD-OE2	9.55	1.36	1.25
2	F	358	ALA	CA-CB	9.55	1.72	1.52
2	J	376	GLU	CD-OE1	9.54	1.36	1.25
1	G	176	GLU	CD-OE2	9.52	1.36	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	408	GLU	CD-OE2	9.39	1.35	1.25
1	K	78	GLU	CD-OE1	9.37	1.35	1.25
1	K	192	GLU	CG-CD	9.36	1.66	1.51
1	C	79	TYR	CD2-CE2	9.31	1.53	1.39
1	E	16	TYR	CD1-CE1	9.30	1.53	1.39
2	J	438	SER	CB-OG	-9.27	1.30	1.42
1	C	168	GLU	CD-OE2	9.21	1.35	1.25
1	C	47	GLU	CD-OE1	9.21	1.35	1.25
1	G	168	GLU	CD-OE1	9.19	1.35	1.25
1	G	3	GLU	CD-OE2	9.14	1.35	1.25
2	F	390	LYS	CD-CE	9.12	1.74	1.51
2	B	499	GLU	CD-OE1	9.12	1.35	1.25
2	L	303	GLN	CA-CB	9.12	1.74	1.53
2	H	507	LYS	CD-CE	9.10	1.74	1.51
2	L	376	GLU	CB-CG	-9.08	1.34	1.52
1	I	64	ARG	CZ-NH1	9.06	1.44	1.33
2	L	447	TYR	CE2-CZ	8.97	1.50	1.38
2	H	390	LYS	CD-CE	8.92	1.73	1.51
1	C	183	TYR	CB-CG	-8.90	1.38	1.51
1	K	78	GLU	CG-CD	8.90	1.65	1.51
2	F	345	GLU	CD-OE2	-8.90	1.15	1.25
2	D	390	LYS	CD-CE	8.89	1.73	1.51
1	K	162	GLU	CD-OE2	8.88	1.35	1.25
1	C	47	GLU	CD-OE2	8.87	1.35	1.25
2	H	380	VAL	CB-CG2	-8.86	1.34	1.52
2	D	456	TRP	CZ3-CH2	8.85	1.54	1.40
2	J	499	GLU	CD-OE1	8.84	1.35	1.25
1	C	188	ARG	CZ-NH1	8.83	1.44	1.33
2	J	303	GLN	CA-CB	8.82	1.73	1.53
2	F	499	GLU	CD-OE1	8.81	1.35	1.25
2	D	388	TYR	CD1-CE1	8.81	1.52	1.39
2	F	440	ARG	CD-NE	-8.75	1.31	1.46
2	D	369	ASN	CB-CG	8.75	1.71	1.51
1	C	198	PHE	CD1-CE1	8.73	1.56	1.39
2	J	479	TYR	CD2-CE2	8.71	1.52	1.39
1	C	165	GLN	CG-CD	8.70	1.71	1.51
1	G	176	GLU	CD-OE1	8.69	1.35	1.25
2	F	507	LYS	CE-NZ	8.67	1.70	1.49
1	E	176	GLU	CG-CD	8.63	1.64	1.51
1	G	55	VAL	CB-CG2	8.62	1.71	1.52
1	E	163	GLN	CG-CD	8.62	1.70	1.51
1	G	92	PHE	CE2-CZ	8.62	1.53	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	471	ALA	CA-CB	-8.60	1.34	1.52
1	C	66	SER	CB-OG	-8.59	1.31	1.42
2	L	522	ARG	CZ-NH1	8.54	1.44	1.33
1	C	109	VAL	CB-CG1	-8.53	1.34	1.52
2	L	315	TRP	CZ3-CH2	8.50	1.53	1.40
1	I	47	GLU	CD-OE2	8.45	1.34	1.25
2	F	526	VAL	CB-CG2	8.42	1.70	1.52
2	L	523	PHE	CD2-CE2	8.42	1.56	1.39
2	J	532	LYS	CA-CB	8.39	1.72	1.53
2	J	308	PHE	CE1-CZ	8.38	1.53	1.37
1	A	86	GLU	CG-CD	8.37	1.64	1.51
2	F	324	TYR	CG-CD1	8.36	1.50	1.39
1	I	165	GLN	CG-CD	8.33	1.70	1.51
1	E	47	GLU	CD-OE2	8.32	1.34	1.25
2	D	499	GLU	CD-OE1	8.31	1.34	1.25
1	C	99	PHE	CD1-CE1	8.30	1.55	1.39
2	D	440	ARG	CD-NE	-8.26	1.32	1.46
2	F	479	TYR	CZ-OH	-8.25	1.23	1.37
2	H	438	SER	CB-OG	-8.25	1.31	1.42
1	K	168	GLU	CD-OE2	8.24	1.34	1.25
2	H	521	TYR	CD2-CE2	8.23	1.51	1.39
2	L	436	TYR	CD2-CE2	8.23	1.51	1.39
1	K	86	GLU	CD-OE1	8.22	1.34	1.25
2	B	532	LYS	CA-CB	8.21	1.72	1.53
1	K	200	PHE	CG-CD2	8.21	1.51	1.38
1	G	144	TYR	CD2-CE2	8.19	1.51	1.39
2	L	439	PHE	CD1-CE1	8.17	1.55	1.39
2	D	390	LYS	CG-CD	8.09	1.79	1.52
1	E	200	PHE	CB-CG	8.07	1.65	1.51
1	I	183	TYR	CE1-CZ	8.07	1.49	1.38
1	K	196	VAL	CB-CG1	8.06	1.69	1.52
2	J	337	VAL	CB-CG2	8.05	1.69	1.52
1	A	192	GLU	CD-OE2	8.03	1.34	1.25
1	A	114	VAL	CB-CG2	-8.02	1.36	1.52
2	L	324	TYR	CD1-CE1	8.00	1.51	1.39
1	E	86	GLU	CB-CG	7.99	1.67	1.52
2	L	450	ARG	CZ-NH1	7.98	1.43	1.33
1	C	36	TRP	CZ3-CH2	7.97	1.52	1.40
1	C	79	TYR	CD1-CE1	7.95	1.51	1.39
1	I	24	GLU	CD-OE1	7.94	1.34	1.25
2	L	423	PHE	CE2-CZ	7.93	1.52	1.37
1	A	188	ARG	CZ-NH2	7.92	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	333	ARG	CZ-NH2	7.89	1.43	1.33
1	A	154	LYS	CD-CE	7.89	1.71	1.51
1	E	162	GLU	CG-CD	7.88	1.63	1.51
2	L	436	TYR	CD1-CE1	7.87	1.51	1.39
2	B	440	ARG	CD-NE	-7.85	1.33	1.46
1	E	56	TYR	CD2-CE2	7.84	1.51	1.39
2	J	419	LEU	C-O	7.84	1.38	1.23
1	A	131	PHE	CE2-CZ	7.79	1.52	1.37
1	G	78	GLU	CD-OE1	7.78	1.34	1.25
2	F	449	TRP	CZ3-CH2	7.77	1.52	1.40
1	I	56	TYR	CD2-CE2	7.76	1.50	1.39
1	K	38	ARG	CG-CD	7.75	1.71	1.51
2	D	493	LYS	CE-NZ	7.75	1.68	1.49
1	G	176	GLU	CG-CD	7.75	1.63	1.51
1	I	103	GLU	CD-OE2	7.74	1.34	1.25
2	F	480	PHE	CB-CG	-7.73	1.38	1.51
2	B	306	SER	CB-OG	-7.72	1.32	1.42
1	K	183	TYR	CD2-CE2	7.71	1.50	1.39
1	A	163	GLN	CG-CD	7.70	1.68	1.51
1	A	196	VAL	CB-CG1	7.70	1.69	1.52
2	D	521	TYR	CD1-CE1	7.70	1.50	1.39
1	I	192	GLU	CG-CD	7.69	1.63	1.51
1	G	103	GLU	CB-CG	-7.67	1.37	1.52
2	F	318	LYS	CE-NZ	7.67	1.68	1.49
1	G	103	GLU	CD-OE1	7.65	1.34	1.25
2	L	415	TYR	CG-CD2	7.63	1.49	1.39
2	H	450	ARG	CZ-NH2	7.62	1.43	1.33
2	F	415	TYR	CE1-CZ	7.61	1.48	1.38
1	K	3	GLU	CD-OE2	7.61	1.34	1.25
1	I	162	GLU	CG-CD	7.60	1.63	1.51
2	L	415	TYR	CE1-CZ	7.59	1.48	1.38
1	A	168	GLU	CD-OE2	7.59	1.33	1.25
1	I	24	GLU	CG-CD	7.57	1.63	1.51
2	F	520	ALA	CA-CB	-7.57	1.36	1.52
2	F	402	ALA	CA-CB	7.54	1.68	1.52
1	I	163	GLN	CG-CD	7.52	1.68	1.51
2	H	367	PHE	CG-CD1	7.51	1.50	1.38
1	K	101	ALA	CA-CB	7.51	1.68	1.52
2	H	518	CYS	CB-SG	-7.48	1.69	1.82
2	B	493	LYS	CG-CD	7.46	1.77	1.52
2	J	415	TYR	CE2-CZ	7.45	1.48	1.38
2	H	303	GLN	CA-CB	7.41	1.70	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	71	TRP	CE3-CZ3	7.41	1.51	1.38
1	A	3	GLU	CD-OE2	7.40	1.33	1.25
1	I	192	GLU	CD-OE1	7.39	1.33	1.25
1	A	192	GLU	CD-OE1	7.39	1.33	1.25
1	E	192	GLU	CD-OE2	7.36	1.33	1.25
1	A	194	GLU	CD-OE1	-7.34	1.17	1.25
1	E	153	ALA	CA-CB	7.30	1.67	1.52
2	L	376	GLU	CD-OE1	7.29	1.33	1.25
2	J	439	PHE	CE2-CZ	7.28	1.51	1.37
1	K	163	GLN	CG-CD	7.28	1.67	1.51
2	H	352	SER	CB-OG	-7.26	1.32	1.42
1	A	200	PHE	CG-CD1	7.25	1.49	1.38
1	K	86	GLU	CD-OE2	7.25	1.33	1.25
1	K	168	GLU	CD-OE1	7.25	1.33	1.25
1	I	47	GLU	CD-OE1	7.24	1.33	1.25
2	B	436	TYR	CD2-CE2	7.24	1.50	1.39
2	D	523	PHE	CE1-CZ	7.22	1.51	1.37
2	H	502	GLN	CB-CG	7.21	1.72	1.52
1	I	78	GLU	CD-OE1	7.19	1.33	1.25
1	I	16	TYR	CD1-CE1	7.18	1.50	1.39
2	J	342	SER	CB-OG	7.18	1.51	1.42
1	K	168	GLU	CB-CG	7.17	1.65	1.52
1	A	56	TYR	CE1-CZ	7.13	1.47	1.38
1	A	165	GLN	CG-CD	7.13	1.67	1.51
2	B	414	ARG	CB-CG	7.12	1.71	1.52
2	B	327	SER	N-CA	-7.12	1.32	1.46
2	H	405	GLY	C-O	7.12	1.35	1.23
1	G	154	LYS	CE-NZ	7.11	1.66	1.49
2	H	426	VAL	CB-CG2	-7.11	1.38	1.52
1	E	200	PHE	CE2-CZ	7.10	1.50	1.37
1	A	168	GLU	CG-CD	7.08	1.62	1.51
1	K	99	PHE	CD2-CE2	7.08	1.53	1.39
2	D	315	TRP	CB-CG	-7.07	1.37	1.50
2	L	507	LYS	CE-NZ	7.07	1.66	1.49
1	G	26	ALA	C-O	7.06	1.36	1.23
2	H	337	VAL	CB-CG2	7.04	1.67	1.52
1	E	24	GLU	CD-OE2	7.04	1.33	1.25
2	F	433	SER	CA-CB	7.04	1.63	1.52
1	I	25	ALA	CA-CB	-7.03	1.37	1.52
2	J	390	LYS	CD-CE	7.01	1.68	1.51
2	H	388	TYR	CD2-CE2	6.96	1.49	1.39
2	L	333	ARG	CZ-NH1	6.96	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	390	LYS	CG-CD	6.96	1.76	1.52
1	G	64	ARG	CZ-NH1	6.96	1.42	1.33
2	J	333	ARG	CZ-NH1	6.96	1.42	1.33
2	F	345	GLU	CG-CD	6.95	1.62	1.51
2	H	439	PHE	CE2-CZ	6.95	1.50	1.37
1	K	64	ARG	CZ-NH1	6.95	1.42	1.33
2	L	333	ARG	CZ-NH2	6.95	1.42	1.33
1	I	7	GLU	CG-CD	6.94	1.62	1.51
2	D	303	GLN	CA-CB	6.93	1.69	1.53
1	I	24	GLU	CD-OE2	6.92	1.33	1.25
1	K	162	GLU	CG-CD	6.91	1.62	1.51
1	E	86	GLU	CD-OE2	6.91	1.33	1.25
1	C	99	PHE	CD2-CE2	6.90	1.53	1.39
1	I	16	TYR	CD2-CE2	6.90	1.49	1.39
1	C	24	GLU	CD-OE1	6.89	1.33	1.25
2	D	333	ARG	CZ-NH2	6.88	1.42	1.33
1	I	99	PHE	CE2-CZ	6.87	1.50	1.37
1	E	67	PHE	CE2-CZ	6.83	1.50	1.37
2	F	532	LYS	CA-CB	6.83	1.69	1.53
2	H	436	TYR	CD2-CE2	6.83	1.49	1.39
2	J	368	ASN	CB-CG	6.83	1.66	1.51
2	H	403	ASN	C-O	6.82	1.36	1.23
1	G	99	PHE	CE1-CZ	6.82	1.50	1.37
1	I	162	GLU	CD-OE1	6.79	1.33	1.25
1	E	10	SER	CB-OG	-6.79	1.33	1.42
2	L	516	MET	CG-SD	6.78	1.98	1.81
2	B	390	LYS	CD-CE	6.77	1.68	1.51
1	A	67	PHE	CE2-CZ	6.76	1.50	1.37
1	E	142	ARG	CZ-NH1	6.76	1.41	1.33
2	J	335	ALA	CA-CB	6.75	1.66	1.52
2	L	507	LYS	CD-CE	6.75	1.68	1.51
2	D	345	GLU	CG-CD	6.74	1.62	1.51
2	H	439	PHE	CB-CG	-6.72	1.40	1.51
1	E	145	PHE	CE2-CZ	6.71	1.50	1.37
1	A	191	GLY	C-O	6.70	1.34	1.23
2	J	310	ILE	C-O	6.68	1.36	1.23
1	G	163	GLN	CG-CD	6.68	1.66	1.51
2	B	305	ASN	CB-CG	6.67	1.66	1.51
1	C	16	TYR	CD2-CE2	6.67	1.49	1.39
1	C	101	ALA	C-N	6.67	1.45	1.33
1	K	192	GLU	CD-OE2	6.67	1.32	1.25
2	L	408	GLU	CD-OE2	6.67	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	103	GLU	CB-CG	-6.65	1.39	1.52
1	K	104	TRP	CE3-CZ3	6.65	1.49	1.38
1	E	165	GLN	CG-CD	6.64	1.66	1.51
1	K	131	PHE	CE2-CZ	6.64	1.50	1.37
2	B	507	LYS	CE-NZ	6.64	1.65	1.49
2	L	345	GLU	CG-CD	6.64	1.61	1.51
2	B	499	GLU	CD-OE2	6.64	1.32	1.25
1	C	16	TYR	CE2-CZ	6.61	1.47	1.38
1	G	34	GLU	CG-CD	6.61	1.61	1.51
2	H	450	ARG	CZ-NH1	6.60	1.41	1.33
2	L	440	ARG	CD-NE	-6.60	1.35	1.46
1	E	63	VAL	CB-CG2	6.60	1.66	1.52
1	I	35	ILE	CB-CG2	-6.59	1.32	1.52
1	A	99	PHE	CD1-CE1	6.59	1.52	1.39
2	J	466	SER	CB-OG	6.58	1.50	1.42
2	B	493	LYS	CE-NZ	6.57	1.65	1.49
1	K	3	GLU	CD-OE1	6.57	1.32	1.25
2	F	408	GLU	CD-OE1	6.55	1.32	1.25
1	E	86	GLU	CG-CD	6.54	1.61	1.51
2	H	333	ARG	CB-CG	6.54	1.70	1.52
2	F	368	ASN	CB-CG	6.54	1.66	1.51
2	D	450	ARG	CZ-NH1	6.54	1.41	1.33
1	C	177	VAL	CB-CG2	-6.53	1.39	1.52
2	L	414	ARG	CB-CG	6.52	1.70	1.52
2	H	436	TYR	CD1-CE1	6.51	1.49	1.39
2	H	534	HIS	C-O	6.50	1.35	1.23
2	F	411	LYS	CD-CE	6.50	1.67	1.51
1	K	165	GLN	CG-CD	6.50	1.66	1.51
1	I	43	ASP	CB-CG	6.48	1.65	1.51
1	E	144	TYR	CG-CD1	6.47	1.47	1.39
2	B	463	PHE	CB-CG	-6.46	1.40	1.51
1	C	102	GLY	N-CA	6.46	1.55	1.46
1	C	154	LYS	CD-CE	6.46	1.67	1.51
2	B	447	TYR	CG-CD1	6.45	1.47	1.39
2	D	450	ARG	CZ-NH2	6.45	1.41	1.33
1	G	86	GLU	CG-CD	6.44	1.61	1.51
2	B	400	TRP	CE3-CZ3	6.43	1.49	1.38
2	J	449	TRP	CB-CG	6.43	1.61	1.50
1	E	16	TYR	CD2-CE2	6.43	1.49	1.39
2	H	415	TYR	CE1-CZ	6.43	1.47	1.38
2	D	414	ARG	CB-CG	6.42	1.69	1.52
1	E	70	VAL	CB-CG2	-6.41	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	78	GLU	CB-CG	6.41	1.64	1.52
2	J	481	GLU	CB-CG	-6.40	1.40	1.52
2	D	376	GLU	CB-CG	-6.39	1.40	1.52
2	B	507	LYS	CD-CE	6.38	1.67	1.51
1	G	16	TYR	CE2-CZ	6.36	1.46	1.38
2	B	370	GLY	C-O	6.36	1.33	1.23
1	I	47	GLU	CB-CG	6.36	1.64	1.52
2	F	463	PHE	CD1-CE1	6.36	1.51	1.39
2	H	383	ARG	CB-CG	-6.36	1.35	1.52
2	J	521	TYR	CG-CD1	6.35	1.47	1.39
1	E	176	GLU	CD-OE1	6.34	1.32	1.25
1	I	78	GLU	CD-OE2	6.34	1.32	1.25
2	H	516	MET	CA-CB	6.34	1.67	1.53
1	C	36	TRP	CG-CD1	6.34	1.45	1.36
1	E	180	LYS	CE-NZ	6.33	1.64	1.49
2	B	481	GLU	CB-CG	-6.33	1.40	1.52
1	I	83	TYR	CD1-CE1	-6.33	1.29	1.39
1	I	47	GLU	CG-CD	6.32	1.61	1.51
1	E	148	GLU	CB-CG	-6.31	1.40	1.52
2	H	530	GLN	CG-CD	6.30	1.65	1.51
2	L	369	ASN	C-O	6.30	1.35	1.23
2	D	532	LYS	CA-CB	6.29	1.67	1.53
2	F	522	ARG	CZ-NH2	6.29	1.41	1.33
1	G	192	GLU	CD-OE2	6.29	1.32	1.25
1	E	47	GLU	CG-CD	6.28	1.61	1.51
1	A	197	PHE	CD1-CE1	6.28	1.51	1.39
1	K	176	GLU	CG-CD	6.27	1.61	1.51
2	H	408	GLU	CG-CD	-6.26	1.42	1.51
1	K	200	PHE	CE1-CZ	6.26	1.49	1.37
1	C	144	TYR	CE1-CZ	6.26	1.46	1.38
2	D	521	TYR	CD2-CE2	6.26	1.48	1.39
1	G	168	GLU	CG-CD	6.25	1.61	1.51
2	J	381	ALA	CA-CB	-6.25	1.39	1.52
2	F	303	GLN	CA-CB	6.25	1.67	1.53
2	D	441	THR	CB-CG2	6.25	1.73	1.52
2	H	358	ALA	CA-CB	6.24	1.65	1.52
2	F	376	GLU	CG-CD	6.24	1.61	1.51
1	C	98	THR	N-CA	6.23	1.58	1.46
2	J	523	PHE	CE1-CZ	6.23	1.49	1.37
2	D	457	ARG	CZ-NH2	-6.21	1.25	1.33
1	A	162	GLU	CG-CD	6.20	1.61	1.51
1	I	174	ARG	CZ-NH2	6.20	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	528	ARG	CZ-NH1	6.19	1.41	1.33
1	K	184	ARG	CZ-NH2	6.19	1.41	1.33
2	B	528	ARG	CB-CG	6.18	1.69	1.52
2	J	377	ARG	CB-CG	6.18	1.69	1.52
1	K	145	PHE	CE1-CZ	6.18	1.49	1.37
1	I	34	GLU	CD-OE1	6.17	1.32	1.25
1	I	103	GLU	CD-OE1	6.17	1.32	1.25
2	J	376	GLU	CG-CD	6.17	1.61	1.51
1	G	192	GLU	CB-CG	6.16	1.63	1.52
2	H	449	TRP	CZ3-CH2	6.16	1.50	1.40
2	F	376	GLU	CD-OE1	6.15	1.32	1.25
1	G	188	ARG	CZ-NH2	6.15	1.41	1.33
1	K	114	VAL	CA-CB	6.15	1.67	1.54
2	L	387	GLN	CB-CG	-6.14	1.35	1.52
1	I	149	ALA	CA-CB	6.13	1.65	1.52
2	J	450	ARG	CZ-NH2	6.11	1.41	1.33
1	E	96	ALA	CA-CB	6.11	1.65	1.52
1	G	30	THR	CB-CG2	6.11	1.72	1.52
2	H	308	PHE	CD1-CE1	6.10	1.51	1.39
1	K	142	ARG	CZ-NH1	6.10	1.41	1.33
2	J	388	TYR	CE2-CZ	6.10	1.46	1.38
2	J	449	TRP	C-O	6.10	1.34	1.23
1	K	34	GLU	CG-CD	6.09	1.61	1.51
2	J	480	PHE	CE1-CZ	6.09	1.49	1.37
2	D	437	TYR	CE2-CZ	6.08	1.46	1.38
2	D	473	LYS	CD-CE	6.08	1.66	1.51
2	L	327	SER	N-CA	-6.08	1.34	1.46
2	D	458	PRO	CA-C	6.07	1.65	1.52
1	A	63	VAL	CB-CG1	-6.07	1.40	1.52
1	C	24	GLU	CD-OE2	6.06	1.32	1.25
2	F	403	ASN	C-O	6.06	1.34	1.23
1	E	55	VAL	CB-CG2	6.06	1.65	1.52
2	B	315	TRP	CG-CD1	-6.06	1.28	1.36
2	D	414	ARG	CZ-NH1	6.05	1.41	1.33
1	G	92	PHE	CG-CD1	6.05	1.47	1.38
1	E	142	ARG	CZ-NH2	6.05	1.41	1.33
1	K	64	ARG	CG-CD	6.05	1.67	1.51
1	C	100	ASP	CB-CG	6.04	1.64	1.51
2	H	390	LYS	CG-CD	6.04	1.73	1.52
1	I	176	GLU	CD-OE2	6.04	1.32	1.25
2	H	381	ALA	CA-CB	-6.03	1.39	1.52
1	G	144	TYR	CG-CD1	6.02	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	78	GLU	CB-CG	6.02	1.63	1.52
2	J	521	TYR	CE2-CZ	6.02	1.46	1.38
1	C	63	VAL	CB-CG2	-6.01	1.40	1.52
2	D	537	ASN	CB-CG	5.99	1.64	1.51
2	H	367	PHE	CE1-CZ	5.99	1.48	1.37
1	I	192	GLU	CD-OE2	5.99	1.32	1.25
2	B	428	ARG	CD-NE	-5.99	1.36	1.46
2	L	456	TRP	CE3-CZ3	-5.99	1.28	1.38
1	A	188	ARG	CZ-NH1	5.98	1.40	1.33
2	D	521	TYR	CG-CD2	5.98	1.47	1.39
1	G	165	GLN	CG-CD	5.98	1.64	1.51
2	L	409	ARG	CZ-NH2	5.96	1.40	1.33
1	G	192	GLU	CG-CD	5.96	1.60	1.51
2	J	449	TRP	CG-CD1	5.95	1.45	1.36
1	C	78	GLU	CD-OE1	5.93	1.32	1.25
2	L	414	ARG	CZ-NH2	5.93	1.40	1.33
2	B	365	LEU	C-O	-5.92	1.12	1.23
1	K	86	GLU	CG-CD	5.92	1.60	1.51
2	J	440	ARG	C-O	5.91	1.34	1.23
1	A	94	ARG	CD-NE	-5.91	1.36	1.46
1	K	179	GLY	C-O	5.91	1.33	1.23
2	L	537	ASN	N-CA	5.90	1.58	1.46
2	L	400	TRP	CE3-CZ3	5.90	1.48	1.38
1	E	183	TYR	CE1-CZ	5.90	1.46	1.38
2	H	481	GLU	CD-OE1	-5.89	1.19	1.25
1	I	131	PHE	CE2-CZ	5.88	1.48	1.37
1	G	14	GLY	C-O	5.88	1.33	1.23
1	I	64	ARG	CZ-NH2	5.87	1.40	1.33
1	C	36	TRP	CD2-CE2	5.87	1.48	1.41
1	E	114	VAL	CB-CG2	-5.86	1.40	1.52
1	E	162	GLU	CD-OE2	5.86	1.32	1.25
2	L	356	PHE	CE1-CZ	5.86	1.48	1.37
1	A	32	ASP	CB-CG	5.86	1.64	1.51
1	C	144	TYR	CD2-CE2	5.86	1.48	1.39
1	K	176	GLU	CB-CG	5.86	1.63	1.52
2	D	345	GLU	CD-OE2	-5.85	1.19	1.25
2	B	502	GLN	CD-OE1	5.85	1.36	1.24
1	A	148	GLU	CD-OE2	-5.85	1.19	1.25
1	I	197	PHE	CE2-CZ	5.84	1.48	1.37
2	H	446	PRO	C-O	5.83	1.34	1.23
2	J	351	PHE	CG-CD1	5.83	1.47	1.38
1	E	22	ALA	CA-CB	5.83	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	99	PHE	CD1-CE1	5.82	1.50	1.39
2	J	507	LYS	CD-CE	5.82	1.65	1.51
2	L	430	LEU	CG-CD2	5.81	1.73	1.51
2	B	379	ILE	CA-CB	-5.81	1.41	1.54
1	A	161	ILE	CA-CB	-5.80	1.41	1.54
1	I	199	ASP	C-O	5.80	1.34	1.23
1	A	31	ARG	CZ-NH2	5.80	1.40	1.33
1	G	157	VAL	CB-CG2	5.80	1.65	1.52
1	G	192	GLU	CD-OE1	5.80	1.32	1.25
2	F	522	ARG	CZ-NH1	5.80	1.40	1.33
1	I	101	ALA	C-N	5.80	1.43	1.33
1	A	47	GLU	CB-CG	5.79	1.63	1.52
2	H	423	PHE	CE2-CZ	5.79	1.48	1.37
1	G	198	PHE	CB-CG	5.79	1.61	1.51
1	C	150	GLN	CD-OE1	5.78	1.36	1.24
1	E	3	GLU	CD-OE2	5.78	1.32	1.25
2	L	521	TYR	CE2-CZ	5.78	1.46	1.38
2	D	489	CYS	CB-SG	-5.77	1.72	1.81
2	B	440	ARG	CG-CD	-5.76	1.37	1.51
2	B	454	ASN	CB-CG	5.75	1.64	1.51
2	J	537	ASN	N-CA	5.75	1.57	1.46
1	E	36	TRP	CZ3-CH2	5.75	1.49	1.40
2	J	492	VAL	CB-CG1	-5.75	1.40	1.52
2	L	345	GLU	CD-OE1	5.74	1.31	1.25
1	C	192	GLU	CD-OE1	5.74	1.31	1.25
1	I	99	PHE	CD1-CE1	5.74	1.50	1.39
2	H	388	TYR	CG-CD2	5.74	1.46	1.39
1	A	64	ARG	CZ-NH1	5.73	1.40	1.33
1	K	109	VAL	CA-CB	5.73	1.66	1.54
1	A	109	VAL	CB-CG2	-5.73	1.40	1.52
2	F	370	GLY	C-O	5.72	1.32	1.23
1	I	154	LYS	CD-CE	5.72	1.65	1.51
2	B	493	LYS	CD-CE	5.72	1.65	1.51
2	B	403	ASN	CG-ND2	5.72	1.47	1.32
2	L	308	PHE	CD2-CE2	5.72	1.50	1.39
2	F	466	SER	CB-OG	5.71	1.49	1.42
1	G	83	TYR	CE1-CZ	5.71	1.46	1.38
1	C	106	LEU	CA-CB	-5.71	1.40	1.53
1	I	99	PHE	CE1-CZ	5.71	1.48	1.37
1	C	35	ILE	CA-CB	-5.71	1.41	1.54
1	I	144	TYR	CE2-CZ	5.70	1.46	1.38
1	K	197	PHE	CE2-CZ	5.70	1.48	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	150	GLN	CD-OE1	5.70	1.36	1.24
1	K	198	PHE	CB-CG	-5.69	1.41	1.51
2	B	414	ARG	NE-CZ	5.68	1.40	1.33
2	L	449	TRP	CZ2-CH2	5.68	1.48	1.37
1	G	40	ALA	CA-CB	-5.68	1.40	1.52
1	G	189	ILE	CA-C	-5.68	1.38	1.52
2	H	447	TYR	CE2-CZ	5.68	1.46	1.38
1	K	188	ARG	CZ-NH1	5.68	1.40	1.33
1	A	145	PHE	CG-CD1	5.67	1.47	1.38
1	G	66	SER	CB-OG	-5.67	1.34	1.42
2	D	423	PHE	CB-CG	-5.67	1.41	1.51
2	B	518	CYS	CB-SG	-5.66	1.72	1.81
1	I	198	PHE	CD2-CE2	5.66	1.50	1.39
2	H	502	GLN	CD-OE1	5.66	1.36	1.24
2	B	438	SER	CB-OG	-5.66	1.34	1.42
1	E	197	PHE	CG-CD1	5.66	1.47	1.38
1	G	200	PHE	CB-CG	-5.65	1.41	1.51
2	J	368	ASN	C-O	5.65	1.34	1.23
2	L	384	VAL	CB-CG1	-5.65	1.41	1.52
2	J	499	GLU	CD-OE2	5.64	1.31	1.25
2	L	415	TYR	CZ-OH	-5.63	1.28	1.37
2	B	367	PHE	CE1-CZ	5.63	1.48	1.37
2	H	383	ARG	CZ-NH2	5.63	1.40	1.33
1	E	99	PHE	CE1-CZ	5.62	1.48	1.37
1	A	166	ARG	CZ-NH1	5.62	1.40	1.33
2	B	454	ASN	C-O	5.61	1.34	1.23
1	K	24	GLU	CD-OE2	5.61	1.31	1.25
2	B	320	LEU	C-O	-5.61	1.12	1.23
1	I	15	PRO	C-O	-5.61	1.12	1.23
1	I	67	PHE	CG-CD1	5.60	1.47	1.38
1	E	168	GLU	CD-OE2	5.60	1.31	1.25
2	H	449	TRP	CD2-CE2	5.60	1.48	1.41
2	F	368	ASN	N-CA	5.60	1.57	1.46
2	H	414	ARG	CZ-NH1	5.60	1.40	1.33
1	C	13	ALA	N-CA	5.60	1.57	1.46
1	A	83	TYR	CG-CD1	-5.59	1.31	1.39
1	E	174	ARG	CZ-NH1	5.59	1.40	1.33
2	F	437	TYR	C-O	5.59	1.33	1.23
1	G	63	VAL	CB-CG1	-5.59	1.41	1.52
1	K	155	CYS	C-O	5.58	1.33	1.23
1	C	64	ARG	CZ-NH1	5.58	1.40	1.33
2	F	352	SER	CB-OG	-5.58	1.34	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	168	GLU	CG-CD	5.58	1.60	1.51
1	G	200	PHE	CE2-CZ	5.57	1.48	1.37
1	C	38	ARG	CB-CG	-5.57	1.37	1.52
2	L	351	PHE	CE2-CZ	5.57	1.48	1.37
2	H	481	GLU	CB-CG	-5.56	1.41	1.52
2	B	522	ARG	CG-CD	5.56	1.65	1.51
1	E	35	ILE	CB-CG2	-5.56	1.35	1.52
1	G	7	GLU	CD-OE2	5.56	1.31	1.25
2	H	308	PHE	CE1-CZ	5.56	1.48	1.37
2	J	507	LYS	CE-NZ	5.56	1.62	1.49
2	D	522	ARG	CZ-NH1	5.55	1.40	1.33
1	E	38	ARG	CG-CD	5.55	1.65	1.51
2	D	409	ARG	CB-CG	-5.54	1.37	1.52
2	B	303	GLN	CA-CB	5.53	1.66	1.53
2	D	454	ASN	CB-CG	5.53	1.63	1.51
1	G	15	PRO	CA-C	-5.53	1.41	1.52
2	D	318	LYS	CE-NZ	5.53	1.62	1.49
2	F	507	LYS	CD-CE	5.53	1.65	1.51
2	H	384	VAL	CB-CG2	5.53	1.64	1.52
2	L	414	ARG	NE-CZ	5.52	1.40	1.33
1	E	103	GLU	CD-OE1	5.51	1.31	1.25
2	B	439	PHE	CE2-CZ	5.51	1.47	1.37
1	I	108	THR	C-O	-5.51	1.12	1.23
2	B	530	GLN	CG-CD	5.50	1.63	1.51
1	E	3	GLU	CG-CD	-5.50	1.43	1.51
2	B	369	ASN	C-O	5.50	1.33	1.23
1	E	150	GLN	CG-CD	5.50	1.63	1.51
2	J	400	TRP	CE3-CZ3	5.50	1.47	1.38
2	F	461	ILE	C-O	-5.49	1.12	1.23
2	L	339	ILE	C-O	5.49	1.33	1.23
1	G	56	TYR	CE1-CZ	5.49	1.45	1.38
1	C	67	PHE	CE2-CZ	5.49	1.47	1.37
1	K	7	GLU	CG-CD	5.48	1.60	1.51
1	E	103	GLU	CD-OE2	5.48	1.31	1.25
2	H	428	ARG	CG-CD	-5.48	1.38	1.51
2	B	440	ARG	CA-CB	-5.47	1.42	1.53
1	I	3	GLU	CD-OE1	5.47	1.31	1.25
1	K	193	GLY	CA-C	5.47	1.60	1.51
2	J	493	LYS	CE-NZ	5.47	1.62	1.49
1	G	83	TYR	CG-CD2	5.46	1.46	1.39
1	A	64	ARG	CZ-NH2	5.46	1.40	1.33
1	A	144	TYR	CE2-CZ	5.46	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	414	ARG	CZ-NH1	5.46	1.40	1.33
2	J	393	PRO	CA-C	-5.45	1.42	1.52
1	K	86	GLU	CB-CG	5.45	1.62	1.52
1	G	198	PHE	CD2-CE2	5.44	1.50	1.39
1	E	78	GLU	CD-OE2	5.43	1.31	1.25
1	C	99	PHE	CG-CD2	5.43	1.46	1.38
2	H	493	LYS	CG-CD	5.42	1.70	1.52
1	A	194	GLU	CD-OE2	-5.42	1.19	1.25
2	F	473	LYS	CG-CD	-5.42	1.34	1.52
2	H	458	PRO	CA-C	5.41	1.63	1.52
1	K	99	PHE	CD1-CE1	5.41	1.50	1.39
2	D	456	TRP	CD2-CE2	5.41	1.47	1.41
1	E	36	TRP	CD2-CE3	5.41	1.48	1.40
2	L	392	VAL	CB-CG1	-5.41	1.41	1.52
2	F	535	PHE	CG-CD2	5.39	1.46	1.38
1	A	141	THR	N-CA	-5.38	1.35	1.46
1	C	16	TYR	CG-CD1	5.38	1.46	1.39
2	D	368	ASN	N-CA	5.38	1.57	1.46
2	L	357	GLY	CA-C	5.38	1.60	1.51
1	E	180	LYS	CD-CE	5.38	1.64	1.51
1	C	165	GLN	CB-CG	5.38	1.67	1.52
1	C	94	ARG	CB-CG	-5.37	1.38	1.52
1	A	84	ASN	CB-CG	5.37	1.63	1.51
2	L	455	ASP	C-O	5.37	1.33	1.23
2	F	423	PHE	C-O	5.36	1.33	1.23
2	B	408	GLU	CB-CG	-5.36	1.42	1.52
1	C	53	GLY	N-CA	-5.36	1.38	1.46
2	D	449	TRP	CD2-CE2	5.36	1.47	1.41
1	C	198	PHE	CD2-CE2	5.36	1.50	1.39
1	I	194	GLU	CB-CG	-5.36	1.42	1.52
1	I	10	SER	CA-CB	5.35	1.60	1.52
1	I	196	VAL	CB-CG2	-5.35	1.41	1.52
2	H	390	LYS	CE-NZ	5.34	1.62	1.49
2	J	502	GLN	CD-OE1	5.34	1.35	1.24
2	L	481	GLU	CD-OE1	-5.34	1.19	1.25
1	C	16	TYR	CD1-CE1	5.34	1.47	1.39
2	B	503	GLN	CD-OE1	5.34	1.35	1.24
2	F	400	TRP	CG-CD1	5.33	1.44	1.36
2	B	436	TYR	CZ-OH	-5.33	1.28	1.37
2	J	376	GLU	CB-CG	-5.33	1.42	1.52
2	J	414	ARG	CB-CG	5.32	1.67	1.52
2	D	390	LYS	CE-NZ	5.32	1.62	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	356	PHE	CE2-CZ	5.32	1.47	1.37
2	J	411	LYS	CD-CE	5.32	1.64	1.51
2	L	345	GLU	CD-OE2	5.32	1.31	1.25
2	H	456	TRP	CE3-CZ3	5.31	1.47	1.38
2	L	520	ALA	C-O	5.31	1.33	1.23
2	F	436	TYR	CG-CD1	5.31	1.46	1.39
2	D	380	VAL	CA-CB	5.31	1.66	1.54
2	B	437	TYR	CD2-CE2	5.31	1.47	1.39
1	E	184	ARG	CZ-NH2	5.31	1.40	1.33
1	K	150	GLN	CD-OE1	5.31	1.35	1.24
1	C	1	PRO	CA-C	5.30	1.63	1.52
1	G	85	LEU	C-O	-5.30	1.13	1.23
2	F	351	PHE	CD1-CE1	5.30	1.49	1.39
1	G	180	LYS	CD-CE	5.30	1.64	1.51
1	K	176	GLU	CD-OE2	5.30	1.31	1.25
2	F	365	LEU	C-O	-5.29	1.13	1.23
1	I	54	GLN	C-O	5.29	1.33	1.23
1	C	81	ASP	CA-CB	-5.28	1.42	1.53
2	J	333	ARG	CZ-NH2	5.28	1.40	1.33
1	C	92	PHE	CD2-CE2	5.28	1.49	1.39
2	F	376	GLU	CD-OE2	5.27	1.31	1.25
2	H	313	ARG	CB-CG	5.27	1.66	1.52
2	J	367	PHE	C-O	5.27	1.33	1.23
1	A	43	ASP	CB-CG	5.26	1.62	1.51
1	C	36	TRP	CE3-CZ3	5.26	1.47	1.38
2	F	439	PHE	CE2-CZ	5.26	1.47	1.37
1	G	3	GLU	CD-OE1	5.26	1.31	1.25
1	E	198	PHE	CB-CG	-5.26	1.42	1.51
1	E	119	GLY	CA-C	5.26	1.60	1.51
2	J	408	GLU	CD-OE2	5.25	1.31	1.25
2	J	421	PRO	CA-C	5.25	1.63	1.52
2	D	476	THR	N-CA	-5.25	1.35	1.46
1	K	67	PHE	CB-CG	-5.25	1.42	1.51
2	L	530	GLN	C-O	5.24	1.33	1.23
2	H	318	LYS	CD-CE	5.24	1.64	1.51
1	G	69	GLU	CD-OE1	5.24	1.31	1.25
2	H	480	PHE	CE2-CZ	5.24	1.47	1.37
2	J	423	PHE	CE1-CZ	5.24	1.47	1.37
2	D	518	CYS	C-O	5.23	1.33	1.23
1	K	26	ALA	C-O	5.23	1.33	1.23
1	A	101	ALA	C-N	5.23	1.42	1.33
1	C	120	VAL	CA-CB	-5.23	1.43	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	98	THR	C-O	5.23	1.33	1.23
1	G	86	GLU	CD-OE1	5.23	1.31	1.25
1	C	36	TRP	CG-CD2	5.23	1.52	1.43
1	C	26	ALA	CA-CB	5.22	1.63	1.52
1	I	129	SER	CB-OG	5.22	1.49	1.42
1	C	98	THR	CA-C	5.22	1.66	1.52
2	J	414	ARG	NE-CZ	5.22	1.39	1.33
2	F	518	CYS	CB-SG	-5.22	1.73	1.81
1	G	197	PHE	CG-CD1	5.22	1.46	1.38
1	G	174	ARG	CZ-NH1	5.22	1.39	1.33
2	D	528	ARG	CZ-NH2	5.21	1.39	1.33
2	D	368	ASN	CA-CB	5.21	1.66	1.53
2	L	314	ASN	CB-CG	5.21	1.63	1.51
1	I	179	GLY	C-O	5.21	1.31	1.23
1	I	188	ARG	CZ-NH1	5.21	1.39	1.33
2	L	439	PHE	CD2-CE2	5.21	1.49	1.39
2	B	476	THR	CB-CG2	5.20	1.69	1.52
1	E	189	ILE	CB-CG2	5.20	1.69	1.52
2	J	414	ARG	CD-NE	5.20	1.55	1.46
2	D	335	ALA	CA-CB	5.19	1.63	1.52
2	F	535	PHE	CD2-CE2	5.19	1.49	1.39
2	J	305	ASN	CB-CG	5.19	1.62	1.51
2	D	423	PHE	CG-CD2	5.17	1.46	1.38
1	E	160	LEU	N-CA	-5.17	1.36	1.46
2	L	401	GLN	C-O	5.17	1.33	1.23
1	E	103	GLU	CB-CG	-5.17	1.42	1.52
1	K	99	PHE	CE1-CZ	5.17	1.47	1.37
1	C	154	LYS	CE-NZ	5.17	1.61	1.49
2	J	501	VAL	CB-CG1	5.17	1.63	1.52
2	B	387	GLN	CB-CG	-5.17	1.38	1.52
1	K	189	ILE	CA-CB	-5.17	1.43	1.54
1	K	25	ALA	CA-CB	-5.16	1.41	1.52
1	E	71	TRP	CG-CD1	5.16	1.44	1.36
2	F	482	GLY	CA-C	5.16	1.60	1.51
2	H	452	GLY	CA-C	5.16	1.60	1.51
2	L	351	PHE	CD1-CE1	5.16	1.49	1.39
2	L	411	LYS	CD-CE	5.16	1.64	1.51
2	F	414	ARG	CZ-NH1	5.15	1.39	1.33
2	J	398	GLU	CD-OE2	5.15	1.31	1.25
1	G	56	TYR	CG-CD2	5.15	1.45	1.39
1	E	200	PHE	CD2-CE2	-5.14	1.28	1.39
2	D	493	LYS	CD-CE	5.14	1.64	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	324	TYR	CE1-CZ	5.13	1.45	1.38
2	L	358	ALA	CA-CB	5.13	1.63	1.52
1	K	154	LYS	CE-NZ	5.13	1.61	1.49
2	L	479	TYR	N-CA	5.13	1.56	1.46
2	B	356	PHE	CE2-CZ	5.13	1.47	1.37
1	K	177	VAL	CB-CG2	5.13	1.63	1.52
1	K	144	TYR	C-O	5.12	1.33	1.23
2	F	480	PHE	CE1-CZ	5.11	1.47	1.37
1	E	188	ARG	CZ-NH1	5.11	1.39	1.33
2	B	326	THR	C-O	-5.11	1.13	1.23
2	D	313	ARG	NE-CZ	5.11	1.39	1.33
1	C	36	TRP	CZ2-CH2	5.11	1.47	1.37
1	A	133	ARG	CB-CG	-5.10	1.38	1.52
2	B	337	VAL	CB-CG1	5.10	1.63	1.52
1	C	157	VAL	CB-CG2	-5.10	1.42	1.52
1	E	20	GLY	CA-C	-5.09	1.43	1.51
2	F	451	ASN	CB-CG	5.09	1.62	1.51
1	K	101	ALA	C-O	5.09	1.33	1.23
1	G	99	PHE	CD1-CE1	5.09	1.49	1.39
1	E	177	VAL	CB-CG1	5.09	1.63	1.52
1	G	180	LYS	CE-NZ	5.09	1.61	1.49
2	J	504	LEU	C-O	5.09	1.33	1.23
1	G	163	GLN	CD-OE1	5.08	1.35	1.24
1	K	153	ALA	CA-CB	5.08	1.63	1.52
2	D	537	ASN	N-CA	5.08	1.56	1.46
2	B	528	ARG	CZ-NH1	5.07	1.39	1.33
1	I	167	ARG	NE-CZ	5.07	1.39	1.33
2	F	502	GLN	CD-OE1	5.07	1.35	1.24
2	D	403	ASN	CB-CG	5.07	1.62	1.51
2	F	538	CYS	CB-SG	-5.06	1.73	1.81
2	H	305	ASN	CB-CG	5.06	1.62	1.51
2	D	536	GLU	CB-CG	-5.06	1.42	1.52
2	B	394	ASN	CB-CG	5.06	1.62	1.51
2	H	356	PHE	CE1-CZ	5.05	1.47	1.37
2	H	376	GLU	CG-CD	5.05	1.59	1.51
2	L	318	LYS	CD-CE	5.05	1.63	1.51
1	K	170	LEU	CG-CD2	5.05	1.70	1.51
1	C	17	VAL	CB-CG2	5.04	1.63	1.52
2	L	453	PRO	C-O	-5.04	1.13	1.23
1	G	120	VAL	CB-CG2	-5.04	1.42	1.52
2	J	334	GLN	N-CA	-5.04	1.36	1.46
2	L	368	ASN	CB-CG	5.04	1.62	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	415	TYR	CG-CD2	5.03	1.45	1.39
2	D	516	MET	CB-CG	5.03	1.67	1.51
2	B	420	ASP	C-O	5.02	1.32	1.23
2	D	414	ARG	CG-CD	5.02	1.64	1.51
2	L	301	PRO	CB-CG	5.02	1.75	1.50
2	B	537	ASN	N-CA	5.01	1.56	1.46
2	F	438	SER	CB-OG	-5.01	1.35	1.42
2	H	351	PHE	CE1-CZ	5.01	1.46	1.37
1	G	23	LEU	CG-CD1	5.01	1.70	1.51
1	E	131	PHE	CE2-CZ	-5.01	1.27	1.37
2	F	324	TYR	C-O	5.01	1.32	1.23
2	F	511	ASN	CB-CG	5.00	1.62	1.51
2	D	414	ARG	NE-CZ	5.00	1.39	1.33
2	F	414	ARG	CZ-NH2	5.00	1.39	1.33
2	J	443	LYS	CE-NZ	5.00	1.61	1.49
2	L	388	TYR	CE1-CZ	5.00	1.45	1.38
1	A	67	PHE	CD2-CE2	-5.00	1.29	1.39

All (401) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	440	ARG	NE-CZ-NH1	23.77	132.19	120.30
1	K	94	ARG	NE-CZ-NH1	22.83	131.72	120.30
1	K	94	ARG	NE-CZ-NH2	-22.73	108.94	120.30
1	C	184	ARG	NE-CZ-NH2	-22.09	109.26	120.30
2	H	440	ARG	NE-CZ-NH2	-21.08	109.76	120.30
1	I	94	ARG	NE-CZ-NH1	20.47	130.53	120.30
2	F	440	ARG	NE-CZ-NH1	19.96	130.28	120.30
1	I	94	ARG	NE-CZ-NH2	-19.39	110.61	120.30
1	C	94	ARG	NE-CZ-NH1	18.62	129.61	120.30
1	C	94	ARG	NE-CZ-NH2	-18.32	111.14	120.30
1	A	94	ARG	NE-CZ-NH2	-18.12	111.24	120.30
1	G	94	ARG	NE-CZ-NH1	17.91	129.25	120.30
2	B	428	ARG	NE-CZ-NH2	-17.85	111.38	120.30
2	H	428	ARG	NE-CZ-NH1	17.82	129.21	120.30
1	G	94	ARG	NE-CZ-NH2	-17.72	111.44	120.30
1	C	184	ARG	NE-CZ-NH1	16.95	128.77	120.30
2	B	538	CYS	CA-CB-SG	-16.79	83.78	114.00
2	F	330	ARG	NE-CZ-NH2	-16.05	112.27	120.30
2	L	440	ARG	NE-CZ-NH2	-16.03	112.29	120.30
2	F	428	ARG	NE-CZ-NH2	-16.02	112.29	120.30
2	J	428	ARG	NE-CZ-NH2	-15.97	112.31	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	440	ARG	NE-CZ-NH2	-15.51	112.55	120.30
2	D	428	ARG	NE-CZ-NH2	-15.45	112.58	120.30
2	L	450	ARG	NE-CZ-NH2	-15.41	112.59	120.30
2	H	538	CYS	CA-CB-SG	-15.28	86.50	114.00
2	J	538	CYS	CA-CB-SG	-15.03	86.95	114.00
2	H	440	ARG	NE-CZ-NH1	14.82	127.71	120.30
2	B	330	ARG	NE-CZ-NH2	-14.66	112.97	120.30
1	A	166	ARG	NE-CZ-NH1	14.31	127.46	120.30
1	K	133	ARG	NE-CZ-NH2	-14.26	113.17	120.30
2	L	428	ARG	NE-CZ-NH1	14.25	127.43	120.30
1	A	94	ARG	NE-CZ-NH1	13.97	127.28	120.30
2	J	428	ARG	NE-CZ-NH1	13.96	127.28	120.30
1	C	133	ARG	NE-CZ-NH2	-13.88	113.36	120.30
2	L	428	ARG	NE-CZ-NH2	-13.85	113.38	120.30
1	A	166	ARG	NE-CZ-NH2	-13.58	113.51	120.30
2	L	538	CYS	CA-CB-SG	-13.55	89.60	114.00
2	F	457	ARG	NE-CZ-NH2	-13.51	113.54	120.30
2	D	538	CYS	CA-CB-SG	-13.24	90.17	114.00
2	F	450	ARG	NE-CZ-NH2	-13.14	113.73	120.30
2	F	440	ARG	NE-CZ-NH2	-13.12	113.74	120.30
2	J	440	ARG	NE-CZ-NH2	-13.01	113.80	120.30
2	D	428	ARG	NE-CZ-NH1	12.79	126.69	120.30
2	F	330	ARG	NE-CZ-NH1	12.77	126.68	120.30
1	C	133	ARG	NE-CZ-NH1	12.61	126.61	120.30
1	K	133	ARG	NE-CZ-NH1	12.49	126.54	120.30
2	B	440	ARG	NE-CZ-NH2	-12.32	114.14	120.30
2	J	440	ARG	NE-CZ-NH1	12.29	126.45	120.30
2	H	450	ARG	NE-CZ-NH1	-12.07	114.26	120.30
2	F	333	ARG	NE-CZ-NH2	-11.97	114.31	120.30
2	B	507	LYS	CD-CE-NZ	11.96	139.21	111.70
2	B	428	ARG	NE-CZ-NH1	11.90	126.25	120.30
2	D	493	LYS	CD-CE-NZ	11.56	138.28	111.70
2	F	538	CYS	CA-CB-SG	-11.52	93.26	114.00
1	C	188	ARG	NE-CZ-NH2	-11.52	114.54	120.30
2	D	457	ARG	NE-CZ-NH2	-11.25	114.68	120.30
1	K	184	ARG	NE-CZ-NH1	-11.18	114.71	120.30
2	B	493	LYS	CD-CE-NZ	10.79	136.51	111.70
1	G	133	ARG	NE-CZ-NH2	-10.76	114.92	120.30
2	H	323	ASP	CB-CG-OD1	10.75	127.97	118.30
1	G	133	ARG	NE-CZ-NH1	10.72	125.66	120.30
1	A	184	ARG	NE-CZ-NH2	-10.64	114.98	120.30
2	D	383	ARG	NE-CZ-NH2	-10.64	114.98	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	457	ARG	NE-CZ-NH1	10.61	125.61	120.30
2	H	428	ARG	NE-CZ-NH2	-10.51	115.05	120.30
1	G	186	ASP	CB-CG-OD1	10.43	127.68	118.30
2	J	522	ARG	NE-CZ-NH1	-10.36	115.12	120.30
1	E	188	ARG	NE-CZ-NH1	10.27	125.43	120.30
1	K	52	LEU	CA-CB-CG	10.24	138.86	115.30
2	F	428	ARG	NE-CZ-NH1	10.17	125.38	120.30
2	F	507	LYS	CD-CE-NZ	10.15	135.05	111.70
2	F	457	ARG	NE-CZ-NH1	10.13	125.36	120.30
1	I	166	ARG	NE-CZ-NH2	-10.03	115.28	120.30
1	I	184	ARG	NE-CZ-NH2	-10.03	115.29	120.30
2	B	457	ARG	NE-CZ-NH2	-10.01	115.29	120.30
1	C	188	ARG	NE-CZ-NH1	10.00	125.30	120.30
2	L	457	ARG	NE-CZ-NH2	-9.99	115.31	120.30
2	F	409	ARG	NE-CZ-NH1	-9.94	115.33	120.30
2	J	457	ARG	NE-CZ-NH2	-9.85	115.38	120.30
2	J	311	ARG	NE-CZ-NH2	-9.84	115.38	120.30
1	I	50	LEU	CB-CG-CD1	-9.75	94.42	111.00
1	I	64	ARG	NE-CZ-NH2	-9.73	115.43	120.30
2	J	440	ARG	CB-CG-CD	-9.73	86.30	111.60
2	J	524	ASP	CB-CG-OD1	9.70	127.03	118.30
1	G	184	ARG	NE-CZ-NH1	9.68	125.14	120.30
2	L	450	ARG	NE-CZ-NH1	9.65	125.13	120.30
2	F	311	ARG	NE-CZ-NH2	-9.62	115.49	120.30
2	B	383	ARG	NE-CZ-NH2	-9.60	115.50	120.30
1	I	133	ARG	NE-CZ-NH2	-9.51	115.55	120.30
1	C	143	LEU	CB-CG-CD1	-9.48	94.89	111.00
2	B	312	ASP	CB-CG-OD1	9.45	126.81	118.30
2	D	440	ARG	NE-CZ-NH1	9.45	125.02	120.30
2	B	434	ASP	CB-CG-OD1	-9.28	109.95	118.30
1	E	180	LYS	CD-CE-NZ	9.12	132.68	111.70
2	D	323	ASP	CB-CG-OD1	9.07	126.46	118.30
1	E	166	ARG	NE-CZ-NH1	8.98	124.79	120.30
1	G	41	LYS	CD-CE-NZ	-8.97	91.06	111.70
1	E	106	LEU	CB-CG-CD2	-8.94	95.81	111.00
2	D	440	ARG	CB-CG-CD	-8.93	88.39	111.60
2	J	377	ARG	NE-CZ-NH1	-8.90	115.85	120.30
1	G	43	ASP	CB-CG-OD2	-8.88	110.31	118.30
1	C	81	ASP	CB-CG-OD1	8.82	126.24	118.30
1	K	166	ARG	NE-CZ-NH1	8.80	124.70	120.30
2	J	333	ARG	NE-CZ-NH2	-8.73	115.94	120.30
1	C	106	LEU	CB-CG-CD2	-8.64	96.31	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	522	ARG	NE-CZ-NH1	-8.63	115.98	120.30
2	F	420	ASP	CB-CG-OD1	8.60	126.03	118.30
2	J	312	ASP	CB-CG-OD1	8.54	125.98	118.30
2	F	333	ARG	NH1-CZ-NH2	8.41	128.65	119.40
1	C	64	ARG	NE-CZ-NH1	-8.32	116.14	120.30
1	E	166	ARG	NE-CZ-NH2	-8.32	116.14	120.30
1	G	65	ASP	CB-CG-OD1	8.32	125.78	118.30
2	H	440	ARG	CB-CG-CD	-8.31	89.98	111.60
1	E	52	LEU	CA-CB-CG	8.30	134.39	115.30
1	C	5	LEU	CB-CG-CD2	-8.29	96.90	111.00
1	G	186	ASP	CB-CG-OD2	-8.29	110.84	118.30
1	C	186	ASP	CB-CG-OD1	8.23	125.71	118.30
1	G	146	ASP	CB-CG-OD2	8.23	125.71	118.30
1	C	168	GLU	OE1-CD-OE2	8.22	133.17	123.30
2	B	450	ARG	NE-CZ-NH1	8.21	124.41	120.30
2	F	440	ARG	CB-CG-CD	-8.08	90.59	111.60
1	G	199	ASP	CB-CG-OD1	-8.05	111.06	118.30
1	C	94	ARG	CD-NE-CZ	8.01	134.82	123.60
1	C	74	ASP	CB-CG-OD1	8.01	125.51	118.30
2	H	416	LEU	CB-CG-CD1	-8.01	97.39	111.00
1	G	147	ASP	CB-CG-OD1	7.95	125.46	118.30
2	F	528	ARG	NE-CZ-NH2	-7.81	116.39	120.30
1	E	188	ARG	NE-CZ-NH2	-7.80	116.40	120.30
2	F	509	ASP	CB-CG-OD1	7.80	125.32	118.30
2	D	362	ASP	CB-CG-OD1	-7.79	111.29	118.30
2	H	428	ARG	CD-NE-CZ	7.76	134.47	123.60
1	I	188	ARG	NE-CZ-NH2	-7.76	116.42	120.30
2	J	507	LYS	CD-CE-NZ	7.75	129.52	111.70
1	A	94	ARG	CD-NE-CZ	7.69	134.36	123.60
2	L	383	ARG	NE-CZ-NH2	-7.66	116.47	120.30
1	K	94	ARG	CD-NE-CZ	7.64	134.29	123.60
2	B	430	LEU	CB-CG-CD2	-7.63	98.03	111.00
2	L	440	ARG	CB-CG-CD	-7.62	91.77	111.60
2	B	311	ARG	NE-CZ-NH1	7.59	124.10	120.30
2	B	304	ASP	CB-CG-OD2	-7.58	111.47	118.30
2	F	313	ARG	NE-CZ-NH1	7.58	124.09	120.30
2	D	414	ARG	NE-CZ-NH1	7.55	124.08	120.30
1	I	94	ARG	CD-NE-CZ	7.55	134.18	123.60
2	H	432	ASP	CB-CG-OD1	7.55	125.10	118.30
1	I	142	ARG	NE-CZ-NH2	-7.51	116.54	120.30
2	F	434	ASP	CB-CG-OD1	-7.50	111.55	118.30
1	C	166	ARG	CG-CD-NE	-7.46	96.12	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	362	ASP	CB-CG-OD2	7.46	125.02	118.30
1	C	52	LEU	CA-CB-CG	7.45	132.43	115.30
2	F	383	ARG	NE-CZ-NH2	-7.45	116.58	120.30
1	C	81	ASP	CB-CG-OD2	-7.42	111.62	118.30
2	F	312	ASP	CB-CG-OD2	-7.40	111.64	118.30
1	G	51	LEU	CB-CG-CD2	-7.40	98.42	111.00
2	L	377	ARG	NE-CZ-NH1	-7.38	116.61	120.30
2	D	414	ARG	NE-CZ-NH2	-7.38	116.61	120.30
2	B	428	ARG	CB-CG-CD	7.32	130.64	111.60
1	K	65	ASP	CB-CG-OD1	7.29	124.86	118.30
1	I	142	ARG	NE-CZ-NH1	7.28	123.94	120.30
2	H	432	ASP	CB-CG-OD2	-7.26	111.77	118.30
2	F	493	LYS	CD-CE-NZ	7.25	128.37	111.70
1	G	52	LEU	CA-CB-CG	7.22	131.90	115.30
2	D	312	ASP	CB-CG-OD1	7.20	124.78	118.30
1	C	146	ASP	CB-CG-OD1	7.20	124.78	118.30
1	G	106	LEU	CB-CG-CD2	-7.18	98.80	111.00
2	F	420	ASP	CB-CG-OD2	-7.16	111.86	118.30
2	D	524	ASP	CB-CG-OD1	7.16	124.74	118.30
2	J	383	ARG	NE-CZ-NH1	-7.16	116.72	120.30
1	A	142	ARG	NE-CZ-NH2	-7.15	116.72	120.30
2	B	440	ARG	CB-CG-CD	-7.11	93.12	111.60
2	F	450	ARG	NE-CZ-NH1	7.11	123.85	120.30
1	K	167	ARG	NE-CZ-NH1	7.10	123.85	120.30
1	A	31	ARG	NE-CZ-NH1	-7.09	116.75	120.30
2	J	386	ASP	CB-CG-OD2	7.08	124.67	118.30
2	H	507	LYS	CD-CE-NZ	7.06	127.94	111.70
2	D	337	VAL	CG1-CB-CG2	7.06	122.19	110.90
2	J	524	ASP	CB-CG-OD2	-7.03	111.98	118.30
2	H	414	ARG	NE-CZ-NH1	7.02	123.81	120.30
2	F	485	LEU	CB-CG-CD2	-6.99	99.12	111.00
2	B	483	ASP	CB-CG-OD1	6.99	124.59	118.30
1	E	94	ARG	NE-CZ-NH1	-6.96	116.82	120.30
2	H	455	ASP	CB-CG-OD2	6.95	124.55	118.30
1	I	38	ARG	NE-CZ-NH2	-6.92	116.84	120.30
1	K	166	ARG	NE-CZ-NH2	-6.92	116.84	120.30
2	B	450	ARG	NE-CZ-NH2	-6.92	116.84	120.30
1	G	64	ARG	NE-CZ-NH1	6.89	123.75	120.30
2	D	330	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	C	178	ASP	CB-CG-OD1	6.86	124.47	118.30
1	K	114	VAL	CG1-CB-CG2	-6.85	99.94	110.90
2	B	505	ILE	CG1-CB-CG2	-6.84	96.34	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	528	ARG	NE-CZ-NH1	-6.82	116.89	120.30
1	C	47	GLU	OE1-CD-OE2	6.77	131.43	123.30
1	I	32	ASP	CB-CG-OD1	-6.77	112.21	118.30
1	A	64	ARG	NE-CZ-NH1	-6.76	116.92	120.30
1	G	180	LYS	CD-CE-NZ	6.76	127.24	111.70
1	I	5	LEU	CB-CG-CD2	-6.75	99.53	111.00
1	C	184	ARG	CD-NE-CZ	6.74	133.04	123.60
2	L	307	ARG	NE-CZ-NH2	-6.74	116.93	120.30
1	C	74	ASP	CB-CG-OD2	-6.74	112.23	118.30
1	I	52	LEU	CA-CB-CG	6.71	130.72	115.30
2	J	501	VAL	CA-CB-CG2	-6.70	100.86	110.90
2	H	450	ARG	NH1-CZ-NH2	6.70	126.77	119.40
2	D	509	ASP	CB-CG-OD2	6.69	124.32	118.30
2	J	432	ASP	CB-CG-OD2	-6.68	112.29	118.30
2	F	333	ARG	NE-CZ-NH1	-6.67	116.96	120.30
2	B	455	ASP	CB-CG-OD2	6.67	124.30	118.30
2	L	386	ASP	CB-CG-OD1	-6.65	112.32	118.30
2	J	450	ARG	NE-CZ-NH1	-6.64	116.98	120.30
2	H	481	GLU	CG-CD-OE2	6.64	131.58	118.30
2	L	464	GLY	N-CA-C	-6.63	96.52	113.10
1	I	184	ARG	NE-CZ-NH1	6.63	123.62	120.30
2	L	447	TYR	CD1-CE1-CZ	-6.61	113.85	119.80
2	B	362	ASP	CB-CG-OD2	6.60	124.24	118.30
2	B	372	LEU	CA-CB-CG	6.58	130.43	115.30
1	A	41	LYS	CD-CE-NZ	-6.57	96.58	111.70
2	L	386	ASP	CB-CG-OD2	6.57	124.21	118.30
1	E	178	ASP	CB-CG-OD2	-6.53	112.42	118.30
2	F	360	ASP	CB-CG-OD2	-6.53	112.42	118.30
2	B	364	LEU	CB-CG-CD1	6.52	122.08	111.00
1	E	186	ASP	CB-CG-OD1	6.52	124.16	118.30
2	H	416	LEU	CA-CB-CG	6.48	130.19	115.30
1	G	114	VAL	CG1-CB-CG2	-6.47	100.55	110.90
1	G	43	ASP	CB-CG-OD1	6.45	124.10	118.30
2	B	386	ASP	CB-CG-OD2	6.44	124.09	118.30
1	I	41	LYS	CD-CE-NZ	-6.43	96.91	111.70
2	J	483	ASP	CB-CG-OD2	-6.42	112.52	118.30
2	D	376	GLU	CG-CD-OE2	-6.41	105.47	118.30
1	E	57	ASP	CB-CG-OD1	6.39	124.05	118.30
1	A	184	ARG	NE-CZ-NH1	6.39	123.49	120.30
2	D	313	ARG	NE-CZ-NH1	6.36	123.48	120.30
2	L	372	LEU	CB-CG-CD1	6.36	121.81	111.00
1	A	94	ARG	CB-CG-CD	6.34	128.08	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	409	ARG	NE-CZ-NH1	6.33	123.47	120.30
2	B	457	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	C	32	ASP	CB-CG-OD1	-6.29	112.64	118.30
2	J	322	PRO	N-CA-C	6.28	128.43	112.10
1	K	32	ASP	CB-CG-OD2	-6.28	112.65	118.30
1	C	94	ARG	CB-CG-CD	6.28	127.92	111.60
1	C	166	ARG	NE-CZ-NH2	-6.27	117.17	120.30
1	I	147	ASP	CB-CG-OD1	6.26	123.94	118.30
1	E	57	ASP	CB-CG-OD2	-6.25	112.67	118.30
2	F	409	ARG	NE-CZ-NH2	6.25	123.43	120.30
1	A	57	ASP	CB-CG-OD1	6.24	123.92	118.30
2	B	312	ASP	CB-CG-OD2	-6.23	112.69	118.30
1	G	184	ARG	NE-CZ-NH2	-6.22	117.19	120.30
2	F	474	LEU	CB-CG-CD1	-6.21	100.44	111.00
2	B	522	ARG	NE-CZ-NH2	-6.21	117.19	120.30
2	H	428	ARG	CB-CG-CD	6.20	127.71	111.60
1	A	5	LEU	CB-CG-CD2	-6.19	100.48	111.00
2	D	420	ASP	CB-CG-OD1	6.18	123.86	118.30
1	G	199	ASP	CB-CG-OD2	6.17	123.86	118.30
2	D	420	ASP	CB-CG-OD2	-6.17	112.75	118.30
2	D	524	ASP	CB-CG-OD2	-6.17	112.75	118.30
2	J	432	ASP	CB-CG-OD1	6.16	123.85	118.30
1	A	194	GLU	OE1-CD-OE2	-6.14	115.93	123.30
2	L	478	LEU	CA-CB-CG	6.14	129.41	115.30
2	D	323	ASP	OD1-CG-OD2	-6.12	111.67	123.30
1	K	174	ARG	NE-CZ-NH1	-6.11	117.25	120.30
2	D	311	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	C	180	LYS	CB-CA-C	6.10	122.60	110.40
1	K	32	ASP	CB-CG-OD1	6.10	123.79	118.30
2	B	365	LEU	CB-CG-CD1	-6.09	100.64	111.00
1	K	106	LEU	CB-CG-CD2	-6.09	100.65	111.00
2	F	536	GLU	OE1-CD-OE2	-6.08	116.00	123.30
2	H	312	ASP	CB-CG-OD1	6.07	123.76	118.30
2	B	360	ASP	CB-CG-OD2	-6.06	112.84	118.30
2	H	408	GLU	OE1-CD-OE2	6.04	130.55	123.30
2	J	416	LEU	CA-CB-CG	6.04	129.20	115.30
1	A	199	ASP	CB-CG-OD2	6.03	123.73	118.30
1	G	3	GLU	OE1-CD-OE2	6.02	130.53	123.30
1	E	3	GLU	OE1-CD-OE2	6.02	130.52	123.30
2	H	458	PRO	CB-CA-C	-6.01	96.98	112.00
2	J	330	ARG	NE-CZ-NH2	-6.00	117.30	120.30
2	B	524	ASP	CB-CG-OD1	6.00	123.70	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	313	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	C	184	ARG	CG-CD-NE	-5.96	99.28	111.80
1	I	174	ARG	NE-CZ-NH1	-5.95	117.32	120.30
2	B	411	LYS	CD-CE-NZ	-5.94	98.04	111.70
2	H	312	ASP	CB-CG-OD2	-5.91	112.98	118.30
1	G	74	ASP	CB-CG-OD2	-5.90	112.99	118.30
1	A	133	ARG	NE-CZ-NH2	-5.89	117.36	120.30
1	A	69	GLU	OE1-CD-OE2	-5.89	116.23	123.30
1	G	4	LEU	CA-CB-CG	5.87	128.80	115.30
2	D	312	ASP	CB-CG-OD2	-5.87	113.02	118.30
2	F	505	ILE	CG1-CB-CG2	-5.85	98.52	111.40
2	F	323	ASP	CB-CG-OD1	5.85	123.56	118.30
1	A	106	LEU	CB-CG-CD2	-5.84	101.07	111.00
2	B	333	ARG	NE-CZ-NH2	-5.82	117.39	120.30
2	H	537	ASN	C-N-CA	5.82	136.24	121.70
1	G	103	GLU	OE1-CD-OE2	5.81	130.27	123.30
1	I	94	ARG	CB-CA-C	-5.80	98.81	110.40
2	B	473	LYS	CD-CE-NZ	-5.79	98.39	111.70
2	H	388	TYR	CZ-CE2-CD2	-5.79	114.59	119.80
2	L	428	ARG	CB-CG-CD	5.79	126.64	111.60
2	J	408	GLU	OE1-CD-OE2	5.76	130.22	123.30
2	D	428	ARG	CB-CG-CD	5.76	126.58	111.60
1	C	168	GLU	CG-CD-OE2	-5.76	106.78	118.30
1	A	133	ARG	NE-CZ-NH1	5.75	123.18	120.30
2	B	377	ARG	NE-CZ-NH1	-5.75	117.42	120.30
2	H	473	LYS	CD-CE-NZ	-5.73	98.53	111.70
2	D	386	ASP	CB-CG-OD2	5.72	123.45	118.30
1	A	51	LEU	CB-CG-CD2	-5.71	101.29	111.00
1	E	70	VAL	CG1-CB-CG2	-5.69	101.80	110.90
1	A	188	ARG	CB-CG-CD	5.67	126.34	111.60
1	I	78	GLU	OE1-CD-OE2	5.63	130.05	123.30
1	G	57	ASP	CB-CG-OD1	5.62	123.36	118.30
1	C	147	ASP	CB-CG-OD2	5.60	123.34	118.30
2	J	383	ARG	CG-CD-NE	-5.58	100.08	111.80
2	L	451	ASN	N-CA-C	-5.58	95.94	111.00
2	H	383	ARG	NE-CZ-NH1	-5.58	117.51	120.30
2	B	450	ARG	CD-NE-CZ	5.58	131.41	123.60
2	L	538	CYS	N-CA-C	5.56	126.02	111.00
2	L	507	LYS	CD-CE-NZ	5.55	124.46	111.70
2	D	386	ASP	CB-CG-OD1	-5.53	113.33	118.30
1	C	7	GLU	OE1-CD-OE2	5.52	129.92	123.30
2	H	527	LEU	CB-CG-CD1	-5.52	101.62	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	447	TYR	CG-CD2-CE2	-5.52	116.89	121.30
2	J	527	LEU	CB-CG-CD1	-5.51	101.64	111.00
2	D	450	ARG	CA-CB-CG	-5.50	101.30	113.40
1	K	94	ARG	CA-CB-CG	5.49	125.49	113.40
2	D	428	ARG	N-CA-CB	5.49	120.48	110.60
2	B	419	LEU	CA-CB-CG	-5.49	102.67	115.30
2	B	450	ARG	CG-CD-NE	-5.49	100.28	111.80
2	F	413	ASP	CB-CG-OD1	5.49	123.24	118.30
2	B	321	THR	N-CA-C	-5.46	96.27	111.00
1	G	175	CYS	CA-CB-SG	5.45	123.81	114.00
1	A	62	LEU	CB-CG-CD1	-5.45	101.74	111.00
2	B	383	ARG	NE-CZ-NH1	5.45	123.02	120.30
1	K	105	THR	OG1-CB-CG2	-5.44	97.49	110.00
2	J	483	ASP	CB-CG-OD1	5.43	123.19	118.30
2	L	413	ASP	CB-CG-OD1	5.43	123.19	118.30
2	J	478	LEU	CA-CB-CG	5.43	127.78	115.30
2	F	457	ARG	CB-CA-C	-5.42	99.56	110.40
1	C	100	ASP	C-N-CA	5.42	135.24	121.70
2	L	428	ARG	CD-NE-CZ	5.41	131.18	123.60
1	A	57	ASP	CB-CG-OD2	-5.41	113.43	118.30
2	D	369	ASN	CB-CA-C	5.41	121.22	110.40
2	L	517	ASP	CB-CG-OD1	5.41	123.17	118.30
2	B	360	ASP	CB-CG-OD1	5.41	123.17	118.30
2	J	451	ASN	N-CA-C	-5.38	96.46	111.00
1	E	65	ASP	CB-CG-OD1	5.38	123.14	118.30
1	E	147	ASP	CB-CG-OD2	5.38	123.14	118.30
1	I	17	VAL	CG1-CB-CG2	5.37	119.50	110.90
2	L	473	LYS	CD-CE-NZ	-5.35	99.39	111.70
2	J	533	THR	OG1-CB-CG2	-5.34	97.72	110.00
2	B	447	TYR	CD1-CE1-CZ	-5.33	115.00	119.80
2	F	440	ARG	NH1-CZ-NH2	-5.33	113.54	119.40
1	A	4	LEU	N-CA-CB	-5.30	99.80	110.40
2	L	311	ARG	NE-CZ-NH2	-5.29	117.65	120.30
2	J	324	TYR	N-CA-C	-5.29	96.73	111.00
1	K	47	GLU	OE1-CD-OE2	5.28	129.63	123.30
1	E	184	ARG	NE-CZ-NH1	-5.28	117.66	120.30
2	F	537	ASN	C-N-CA	5.27	134.88	121.70
2	J	531	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	C	85	LEU	CB-CG-CD1	-5.26	102.06	111.00
2	J	531	ARG	NE-CZ-NH2	-5.26	117.67	120.30
2	H	444	PRO	CA-N-CD	5.25	119.06	111.70
1	I	56	TYR	CB-CG-CD1	-5.25	117.85	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	174	ARG	NE-CZ-NH1	5.25	122.92	120.30
2	H	457	ARG	CB-CA-C	-5.24	99.91	110.40
2	F	451	ASN	N-CA-C	-5.24	96.86	111.00
2	H	383	ARG	CG-CD-NE	-5.24	100.80	111.80
2	B	365	LEU	CB-CG-CD2	5.24	119.90	111.00
1	A	184	ARG	CG-CD-NE	-5.23	100.82	111.80
1	C	186	ASP	CB-CG-OD2	-5.23	113.60	118.30
2	H	493	LYS	CD-CE-NZ	5.23	123.72	111.70
2	J	457	ARG	CB-CA-C	-5.22	99.95	110.40
2	B	428	ARG	N-CA-CB	5.22	120.00	110.60
1	G	64	ARG	NE-CZ-NH2	-5.22	117.69	120.30
2	H	531	ARG	NE-CZ-NH1	5.21	122.90	120.30
2	J	522	ARG	NH1-CZ-NH2	5.21	125.12	119.40
1	C	65	ASP	CB-CG-OD1	5.20	122.98	118.30
1	G	37	ASN	N-CA-C	5.19	125.02	111.00
1	K	157	VAL	CG1-CB-CG2	5.19	119.20	110.90
2	D	307	ARG	NE-CZ-NH1	5.17	122.89	120.30
2	L	531	ARG	NE-CZ-NH1	-5.17	117.72	120.30
2	J	360	ASP	CB-CG-OD1	5.17	122.95	118.30
1	E	41	LYS	CD-CE-NZ	-5.17	99.82	111.70
1	A	67	PHE	CD1-CE1-CZ	-5.15	113.92	120.10
2	L	320	LEU	CB-CG-CD1	-5.15	102.25	111.00
2	H	481	GLU	OE1-CD-OE2	-5.14	117.13	123.30
2	H	436	TYR	CG-CD1-CE1	5.14	125.42	121.30
2	L	522	ARG	NE-CZ-NH2	-5.14	117.73	120.30
2	F	452	GLY	N-CA-C	-5.12	100.29	113.10
2	F	415	TYR	CB-CG-CD1	-5.12	117.93	121.00
1	C	167	ARG	NE-CZ-NH1	-5.12	117.74	120.30
2	F	428	ARG	CB-CG-CD	5.11	124.90	111.60
2	J	318	LYS	CD-CE-NZ	-5.09	100.00	111.70
2	B	516	MET	CG-SD-CE	-5.09	92.06	100.20
1	E	35	ILE	CG1-CB-CG2	-5.08	100.21	111.40
2	B	509	ASP	CB-CG-OD2	5.07	122.87	118.30
2	L	313	ARG	NE-CZ-NH1	5.07	122.83	120.30
2	L	488	MET	CG-SD-CE	-5.05	92.12	100.20
2	J	428	ARG	CD-NE-CZ	5.05	130.67	123.60
2	D	333	ARG	NE-CZ-NH1	-5.04	117.78	120.30
1	C	99	PHE	CA-C-N	-5.04	106.11	117.20
2	H	538	CYS	N-CA-CB	5.03	119.66	110.60
2	L	474	LEU	CB-CG-CD1	-5.03	102.45	111.00
1	A	97	THR	N-CA-C	-5.03	97.42	111.00
1	A	142	ARG	NE-CZ-NH1	5.02	122.81	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	524	ASP	CB-CG-OD1	5.01	122.81	118.30
1	G	196	VAL	CG1-CB-CG2	-5.00	102.89	110.90

There are no chirality outliers.

All (52) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	115	ASN	Mainchain
1	A	144	TYR	Sidechain
1	A	188	ARG	Sidechain
1	A	64	ARG	Mainchain
2	B	318	LYS	Mainchain
2	B	324	TYR	Sidechain
2	B	436	TYR	Sidechain
2	B	533	THR	Mainchain
2	B	534	HIS	Sidechain
1	C	110	LYS	Mainchain
1	C	16	TYR	Sidechain
1	C	174	ARG	Mainchain
1	C	33	GLN	Mainchain
2	D	428	ARG	Sidechain
2	D	437	TYR	Sidechain
2	D	446	PRO	Mainchain
1	E	125	HIS	Mainchain
1	E	188	ARG	Mainchain
1	E	19	ILE	Mainchain
1	E	79	TYR	Sidechain
1	E	81	ASP	Mainchain
2	F	309	VAL	Mainchain
2	F	330	ARG	Mainchain
2	F	341	GLN	Mainchain
2	F	407	ARG	Sidechain
1	G	139	LEU	Mainchain
1	G	144	TYR	Sidechain
1	G	166	ARG	Mainchain
1	G	33	GLN	Mainchain
1	G	56	TYR	Sidechain
2	H	362	ASP	Mainchain
2	H	437	TYR	Sidechain
2	H	438	SER	Mainchain
2	H	440	ARG	Sidechain
2	H	481	GLU	Mainchain

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Mol	Chain	Res	Type	Group
1	I	110	LYS	Mainchain
1	I	131	PHE	Mainchain
1	I	140	HIS	Mainchain
1	I	151	ALA	Mainchain
1	I	154	LYS	Mainchain
1	I	75	ALA	Mainchain
2	J	320	LEU	Mainchain
2	J	437	TYR	Sidechain
2	J	462	HIS	Mainchain
1	K	133	ARG	Mainchain
1	K	184	ARG	Mainchain
1	K	56	TYR	Sidechain
2	L	332	PRO	Mainchain
2	L	399	MET	Mainchain
2	L	421	PRO	Mainchain
2	L	478	LEU	Mainchain
2	L	529	GLY	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1571	0	1499	20	0
1	C	1571	0	1499	18	0
1	E	1571	0	1499	26	0
1	G	1571	0	1499	20	0
1	I	1571	0	1499	21	0
1	K	1571	0	1499	20	0
2	B	1876	0	1822	37	0
2	D	1876	0	1822	27	0
2	F	1876	0	1821	31	0
2	H	1876	0	1822	27	0
2	J	1876	0	1822	32	0
2	L	1876	0	1822	32	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	J	1	0	0	0	0
3	L	1	0	0	0	0
4	B	11	0	4	4	0
4	D	11	0	3	3	0
4	F	11	0	4	8	0
4	H	11	0	4	5	0
4	J	11	0	3	3	0
4	L	11	0	3	4	0
5	A	88	0	0	1	0
5	B	162	0	0	2	0
5	C	88	0	0	2	0
5	D	168	0	0	1	0
5	E	86	0	0	1	0
5	F	163	0	0	2	0
5	G	92	0	0	0	0
5	H	157	0	0	6	0
5	I	87	0	0	1	0
5	J	172	0	0	3	0
5	K	81	0	0	1	0
5	L	168	0	0	3	0
All	All	22266	0	19946	291	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (291) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:390:LYS:CG	2:L:390:LYS:CD	1.76	1.63
2:J:343:ILE:CD1	2:J:343:ILE:CG1	1.74	1.60
2:D:390:LYS:CD	2:D:390:LYS:CG	1.80	1.59
2:B:493:LYS:CG	2:B:493:LYS:CD	1.77	1.58
1:G:154:LYS:CE	1:G:154:LYS:CD	1.77	1.58
2:L:301:PRO:CG	2:L:301:PRO:CB	1.75	1.57
2:B:429:CME:CE	2:B:429:CME:CZ	1.76	1.56
2:F:429:CME:CZ	2:F:429:CME:CE	1.78	1.56
2:D:493:LYS:CE	2:D:493:LYS:NZ	1.68	1.55
2:F:507:LYS:CE	2:F:507:LYS:NZ	1.70	1.54
2:F:318:LYS:CE	2:F:318:LYS:NZ	1.68	1.53
2:H:429:CME:CE	2:H:429:CME:CZ	1.86	1.52
2:B:318:LYS:CE	2:B:318:LYS:NZ	1.75	1.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:532:LYS:CB	2:L:532:LYS:CA	1.84	1.49
2:H:507:LYS:CE	2:H:507:LYS:NZ	1.77	1.46
4:J:4550:DHB:O2	5:J:4678:HOH:O	1.67	1.13
4:H:3550:DHB:O2	5:H:3678:HOH:O	1.77	1.02
1:E:26:ALA:O	2:F:411:LYS:NZ	2.01	0.94
2:D:411:LYS:HB2	2:D:411:LYS:NZ	1.88	0.89
1:A:165:GLN:H	1:A:165:GLN:NE2	1.71	0.89
1:C:165:GLN:H	1:C:165:GLN:HE21	0.90	0.88
1:C:165:GLN:H	1:C:165:GLN:NE2	1.71	0.88
2:J:411:LYS:HZ2	2:J:411:LYS:H	1.21	0.84
1:C:165:GLN:HE21	1:C:165:GLN:N	1.75	0.83
1:I:165:GLN:H	1:I:165:GLN:NE2	1.74	0.83
4:B:550:DHB:O2	5:B:678:HOH:O	2.01	0.77
1:I:165:GLN:H	1:I:165:GLN:HE21	1.29	0.77
2:J:361:HIS:CD2	2:J:361:HIS:H	2.03	0.76
2:J:368:ASN:ND2	2:J:370:GLY:H	1.83	0.76
2:J:411:LYS:H	2:J:411:LYS:NZ	1.83	0.76
2:B:497:ASN:HD22	2:B:499:GLU:H	1.34	0.75
2:J:497:ASN:HD22	2:J:499:GLU:H	1.35	0.74
1:E:15:PRO:HD3	4:F:2550:DHB:C2	2.17	0.73
2:B:429:CME:CZ	2:B:429:CME:SD	2.77	0.72
2:D:411:LYS:HB2	2:D:411:LYS:HZ3	1.54	0.72
1:C:18:HIS:ND1	5:C:1648:HOH:O	2.24	0.71
2:B:361:HIS:CD2	2:B:361:HIS:H	2.07	0.70
1:G:15:PRO:HD3	4:H:3550:DHB:C1	2.21	0.70
4:F:2550:DHB:O2	5:F:2678:HOH:O	2.09	0.70
2:F:364:LEU:HD22	2:F:440:ARG:HD3	1.72	0.70
1:K:15:PRO:HD3	4:L:5550:DHB:C1	2.23	0.69
2:J:343:ILE:CD1	2:J:343:ILE:CB	2.67	0.69
2:H:493:LYS:HE3	5:H:3909:HOH:O	1.93	0.69
1:G:165:GLN:H	1:G:165:GLN:HE21	1.39	0.69
2:B:368:ASN:HD22	2:B:370:GLY:H	1.42	0.68
2:L:416:LEU:HD23	2:L:416:LEU:H	1.59	0.68
4:L:5550:DHB:O2	5:L:5678:HOH:O	2.11	0.68
2:L:361:HIS:CD2	2:L:361:HIS:H	2.12	0.67
1:G:165:GLN:H	1:G:165:GLN:NE2	1.93	0.67
1:C:98:THR:N	1:C:101:ALA:O	2.24	0.67
2:F:497:ASN:HD22	2:F:499:GLU:H	1.44	0.66
2:D:497:ASN:ND2	2:D:499:GLU:H	1.95	0.64
2:F:315:TRP:HZ2	2:F:503:GLN:HE21	1.46	0.64
2:H:376:GLU:OE1	5:H:3665:HOH:O	2.15	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:411:LYS:H	2:H:411:LYS:HZ3	1.45	0.64
1:I:15:PRO:HD3	4:J:4550:DHB:C1	2.27	0.63
2:H:369:ASN:H	2:H:422:ASN:HD22	1.47	0.63
2:D:497:ASN:HD22	2:D:499:GLU:H	1.43	0.63
1:E:15:PRO:HD3	4:F:2550:DHB:C1	2.29	0.62
2:B:493:LYS:CG	2:B:493:LYS:CE	2.77	0.62
2:B:356:PHE:CD1	2:B:428:ARG:HD3	2.35	0.61
1:I:61:HIS:ND1	1:K:163:GLN:HG3	2.15	0.61
2:F:390:LYS:HD3	5:F:2677:HOH:O	2.00	0.61
1:E:25:ALA:HB1	1:E:98:THR:HG21	1.82	0.61
2:D:368:ASN:ND2	2:D:370:GLY:H	1.98	0.61
1:E:50:LEU:O	1:E:182:ALA:HA	2.01	0.61
2:D:411:LYS:HB2	2:D:411:LYS:HZ2	1.66	0.60
2:H:454:ASN:HB2	2:J:310:ILE:HG13	1.83	0.60
2:L:356:PHE:CD1	2:L:428:ARG:HD3	2.37	0.60
1:A:165:GLN:H	1:A:165:GLN:HE21	1.49	0.59
2:D:361:HIS:H	2:D:361:HIS:CD2	2.18	0.59
2:H:361:HIS:H	2:H:361:HIS:CD2	2.21	0.59
2:L:497:ASN:HD22	2:L:499:GLU:H	1.49	0.59
1:A:20:GLY:HA2	2:B:426:VAL:HG13	1.84	0.59
1:A:15:PRO:HD3	4:B:550:DHB:C1	2.32	0.58
1:C:67:PHE:HZ	1:C:94:ARG:HD2	1.67	0.58
1:A:67:PHE:HZ	1:A:94:ARG:HD2	1.69	0.58
2:B:318:LYS:NZ	2:B:318:LYS:CD	2.65	0.58
1:K:143:LEU:C	1:K:143:LEU:HD23	2.24	0.58
2:J:497:ASN:ND2	2:J:499:GLU:H	2.01	0.57
2:B:497:ASN:ND2	2:B:499:GLU:H	2.02	0.57
2:B:368:ASN:ND2	2:B:370:GLY:H	2.02	0.57
1:G:15:PRO:HD3	4:H:3550:DHB:C2	2.35	0.57
2:J:382:GLY:HA2	2:J:522:ARG:HE	1.70	0.57
1:A:65:ASP:OD2	1:A:133:ARG:HD3	2.05	0.56
1:K:39:LEU:N	1:K:39:LEU:HD12	2.19	0.56
2:B:360:ASP:OD2	2:B:428:ARG:HD2	2.04	0.56
2:B:364:LEU:HD22	2:B:440:ARG:HD3	1.87	0.56
1:G:67:PHE:CZ	1:G:94:ARG:HD2	2.41	0.56
1:E:17:VAL:HG13	1:E:18:HIS:N	2.20	0.56
1:A:67:PHE:CZ	1:A:94:ARG:HD2	2.41	0.55
2:F:315:TRP:HZ2	2:F:503:GLN:NE2	2.03	0.55
1:K:98:THR:N	1:K:101:ALA:O	2.27	0.55
2:B:390:LYS:HD2	5:B:677:HOH:O	2.05	0.55
1:E:15:PRO:HB3	1:E:133:ARG:HD2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:400:TRP:HA	2:J:425:GLY:O	2.07	0.55
1:A:163:GLN:HB3	1:A:165:GLN:NE2	2.21	0.55
2:H:497:ASN:HD22	2:H:499:GLU:H	1.53	0.55
1:G:65:ASP:OD2	1:G:133:ARG:HD3	2.07	0.54
2:L:497:ASN:ND2	2:L:499:GLU:H	2.05	0.54
2:L:390:LYS:HE2	5:L:5838:HOH:O	2.07	0.54
2:F:356:PHE:CD1	2:F:428:ARG:HD3	2.43	0.54
2:L:361:HIS:H	2:L:361:HIS:HD2	1.54	0.54
2:J:368:ASN:HD22	2:J:370:GLY:H	1.55	0.54
2:F:497:ASN:ND2	2:F:499:GLU:H	2.05	0.53
1:K:67:PHE:HZ	1:K:94:ARG:HD2	1.73	0.53
2:L:315:TRP:HZ2	2:L:503:GLN:NE2	2.06	0.53
1:G:155:CYS:HB3	1:G:158:LEU:HB2	1.90	0.53
2:J:356:PHE:CE1	2:J:428:ARG:HD3	2.43	0.53
2:J:429:CME:HE2	2:J:438:SER:O	2.09	0.53
2:B:315:TRP:HZ2	2:B:503:GLN:NE2	2.06	0.53
2:F:361:HIS:H	2:F:361:HIS:CD2	2.27	0.53
1:G:133:ARG:HB2	4:H:3550:DHB:O1	2.09	0.53
1:K:15:PRO:HD3	4:L:5550:DHB:C2	2.37	0.53
2:F:368:ASN:HD22	2:F:370:GLY:H	1.57	0.53
1:G:67:PHE:HZ	1:G:94:ARG:HD2	1.74	0.53
1:C:67:PHE:CZ	1:C:94:ARG:HD2	2.42	0.53
1:I:162:GLU:O	1:I:164:PRO:HD3	2.09	0.53
2:H:453:PRO:HB2	2:J:310:ILE:HD12	1.91	0.52
2:B:400:TRP:HA	2:B:425:GLY:O	2.10	0.52
1:K:31:ARG:NH1	2:L:428:ARG:HG2	2.25	0.52
2:D:400:TRP:HA	2:D:425:GLY:O	2.10	0.52
1:E:14:GLY:HA2	4:F:2550:DHB:H2	1.91	0.52
2:J:307:ARG:HG2	2:J:533:THR:HG22	1.92	0.52
2:L:368:ASN:ND2	2:L:370:GLY:H	2.09	0.51
1:G:25:ALA:HB1	1:G:98:THR:HG21	1.93	0.51
1:K:132:ALA:HB3	1:K:135:ILE:HD12	1.92	0.51
2:D:369:ASN:H	2:D:422:ASN:HD22	1.57	0.51
1:K:165:GLN:H	1:K:165:GLN:NE2	2.09	0.51
1:I:143:LEU:C	1:I:143:LEU:HD23	2.30	0.50
1:I:18:HIS:CG	5:I:4648:HOH:O	2.64	0.50
2:H:315:TRP:HZ2	2:H:503:GLN:NE2	2.09	0.50
1:I:6:PRO:HG2	2:J:503:GLN:NE2	2.26	0.50
2:L:416:LEU:HD23	2:L:416:LEU:N	2.26	0.50
2:J:361:HIS:H	2:J:361:HIS:HD2	1.57	0.50
1:K:65:ASP:OD2	1:K:133:ARG:HD3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:493:LYS:CD	2:B:493:LYS:CB	2.81	0.49
1:K:70:VAL:HG21	1:K:106:LEU:HD21	1.94	0.49
2:B:468:PRO:HD2	2:B:472:THR:HG21	1.93	0.49
2:F:368:ASN:ND2	2:F:370:GLY:H	2.11	0.49
2:L:356:PHE:CE1	2:L:428:ARG:HD3	2.47	0.49
1:E:131:PHE:CD2	2:F:475:ILE:HD12	2.47	0.49
2:D:429:CME:SG	2:D:437:TYR:HB2	2.53	0.49
1:A:24:GLU:O	1:A:27:GLY:N	2.37	0.49
1:A:51:LEU:HD12	1:A:106:LEU:HD23	1.95	0.49
1:C:15:PRO:HD3	4:D:1550:DHB:C1	2.43	0.49
2:J:403:ASN:HB2	5:J:4620:HOH:O	2.13	0.49
1:G:50:LEU:O	1:G:182:ALA:HA	2.13	0.49
1:E:31:ARG:NH1	2:F:428:ARG:HG2	2.28	0.48
1:I:98:THR:N	1:I:101:ALA:O	2.39	0.48
2:J:376:GLU:O	2:J:442:ILE:HA	2.13	0.48
1:K:131:PHE:CD2	2:L:475:ILE:HD12	2.48	0.48
1:G:51:LEU:HD12	1:G:106:LEU:HD23	1.94	0.48
2:J:326:THR:HG22	2:J:330:ARG:HD2	1.95	0.48
2:D:478:LEU:C	2:D:478:LEU:HD23	2.33	0.48
2:L:390:LYS:CD	2:L:390:LYS:CB	2.80	0.48
2:B:416:LEU:HD23	2:B:416:LEU:H	1.78	0.48
2:L:324:TYR:OH	4:L:5550:DHB:O1	2.22	0.48
2:J:315:TRP:HZ2	2:J:503:GLN:HE21	1.62	0.48
1:E:165:GLN:H	1:E:165:GLN:NE2	2.12	0.47
2:B:416:LEU:HD23	5:H:3907:HOH:O	2.14	0.47
1:A:165:GLN:H	1:A:165:GLN:CD	2.17	0.47
2:B:369:ASN:N	2:B:369:ASN:HD22	2.12	0.47
1:G:14:GLY:HA2	4:H:3550:DHB:H2	1.95	0.47
2:H:451:ASN:ND2	2:H:490:PRO:HG2	2.29	0.47
2:L:315:TRP:HZ2	2:L:503:GLN:HE21	1.62	0.47
1:E:132:ALA:HB3	1:E:135:ILE:HD12	1.96	0.47
2:H:429:CME:CZ	2:H:429:CME:SD	3.01	0.47
2:H:497:ASN:ND2	2:H:499:GLU:H	2.13	0.47
1:C:133:ARG:HB2	4:D:1550:DHB:O1	2.15	0.47
2:D:359:HIS:O	2:D:366:ASN:HB3	2.15	0.47
1:E:92:PHE:CD1	2:F:349:PRO:HG3	2.50	0.47
1:I:123:ALA:HB3	1:I:144:TYR:CE2	2.50	0.47
2:J:399:MET:HA	2:J:462:HIS:O	2.15	0.47
2:L:411:LYS:HB2	2:L:411:LYS:NZ	2.29	0.47
2:B:356:PHE:CE1	2:B:428:ARG:HD3	2.51	0.46
1:K:67:PHE:CZ	1:K:94:ARG:HD2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:200:PHE:CG	2:F:345:GLU:HG2	2.50	0.46
2:H:315:TRP:HZ2	2:H:503:GLN:HE21	1.64	0.46
2:J:447:TYR:OH	4:J:4550:DHB:O4	2.34	0.46
1:G:15:PRO:HB3	1:G:133:ARG:HD2	1.98	0.46
1:C:131:PHE:CD2	1:C:138:HIS:HB3	2.51	0.46
1:G:92:PHE:CG	2:H:349:PRO:HG3	2.50	0.46
2:D:429:CME:HE2	2:D:438:SER:O	2.16	0.46
2:J:497:ASN:HD21	2:J:499:GLU:HB2	1.81	0.46
2:D:372:LEU:HA	2:D:373:PRO:HD3	1.85	0.45
2:H:447:TYR:HB2	2:H:448:PRO:HD2	1.99	0.45
1:C:198:PHE:HA	2:D:337:VAL:O	2.16	0.45
1:E:39:LEU:HD11	1:E:93:GLY:HA3	1.97	0.45
1:G:143:LEU:C	1:G:143:LEU:HD23	2.36	0.45
2:L:403:ASN:HB2	5:L:5620:HOH:O	2.16	0.45
2:D:390:LYS:CD	2:D:390:LYS:CB	2.80	0.45
1:E:14:GLY:HA2	4:F:2550:DHB:C2	2.46	0.45
2:J:361:HIS:CD2	2:J:361:HIS:N	2.76	0.45
2:H:307:ARG:HA	2:H:307:ARG:HD3	1.77	0.45
2:H:400:TRP:HA	2:H:425:GLY:O	2.17	0.45
2:B:361:HIS:H	2:B:361:HIS:HD2	1.59	0.45
1:C:24:GLU:O	1:C:27:GLY:HA2	2.16	0.45
2:B:457:ARG:NH1	4:B:550:DHB:O4	2.48	0.45
1:C:4:LEU:HD22	2:H:511:ASN:CG	2.38	0.45
2:B:369:ASN:N	2:B:369:ASN:ND2	2.65	0.45
1:E:133:ARG:HB2	4:F:2550:DHB:O1	2.17	0.45
1:I:17:VAL:HG13	1:I:18:HIS:CD2	2.52	0.45
1:A:70:VAL:HG12	1:A:128:ILE:HG12	1.99	0.44
2:L:400:TRP:HA	2:L:425:GLY:O	2.17	0.44
2:J:538:CYS:C	5:J:951:HOH:O	2.56	0.44
2:B:382:GLY:HA3	2:B:523:PHE:O	2.18	0.44
1:E:74:ASP:HB2	5:E:2690:HOH:O	2.18	0.44
2:B:364:LEU:HD22	2:B:440:ARG:CD	2.47	0.44
2:L:364:LEU:HD12	2:L:373:PRO:HG2	1.99	0.44
2:D:368:ASN:HD22	2:D:370:GLY:H	1.64	0.44
2:D:390:LYS:HD3	5:D:1677:HOH:O	2.17	0.44
2:B:356:PHE:HD1	2:B:428:ARG:HD3	1.81	0.43
2:F:324:TYR:OH	4:F:2550:DHB:O1	2.20	0.43
2:F:420:ASP:HA	2:F:421:PRO:HD2	1.83	0.43
2:F:369:ASN:H	2:F:422:ASN:HD22	1.66	0.43
1:A:50:LEU:O	1:A:182:ALA:HA	2.18	0.43
2:B:504:LEU:HD23	2:B:504:LEU:HA	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:51:LEU:HD12	1:E:106:LEU:HD23	2.00	0.43
2:B:364:LEU:HD11	2:B:442:ILE:HG23	2.00	0.43
2:B:416:LEU:CD2	5:H:3907:HOH:O	2.66	0.43
2:F:478:LEU:C	2:F:478:LEU:HD23	2.39	0.43
2:D:364:LEU:HD12	2:D:364:LEU:HA	1.83	0.43
1:K:18:HIS:CG	5:K:5648:HOH:O	2.71	0.43
1:K:131:PHE:CE2	1:K:138:HIS:HB3	2.54	0.43
2:L:497:ASN:HD22	2:L:497:ASN:C	2.22	0.43
1:A:77:GLY:O	1:A:114:VAL:HG12	2.19	0.43
2:D:497:ASN:HD22	2:D:497:ASN:C	2.20	0.43
1:E:70:VAL:HG11	1:E:106:LEU:HD21	2.00	0.43
1:I:191:GLY:O	1:I:194:GLU:HB2	2.19	0.42
2:D:457:ARG:CD	2:D:491:ILE:HD12	2.49	0.42
2:F:411:LYS:NZ	2:F:411:LYS:H	2.18	0.42
1:I:131:PHE:CE2	1:I:138:HIS:HB3	2.54	0.42
2:L:376:GLU:O	2:L:442:ILE:HA	2.20	0.42
1:A:54:GLN:O	1:A:186:ASP:HA	2.19	0.42
1:C:4:LEU:HD22	2:H:511:ASN:OD1	2.19	0.42
2:F:429:CME:CZ	2:F:429:CME:SD	3.01	0.42
1:I:26:ALA:O	2:J:411:LYS:HE3	2.20	0.42
2:L:315:TRP:CZ2	2:L:503:GLN:NE2	2.87	0.42
2:D:476:THR:OG1	2:D:477:GLN:N	2.53	0.42
2:J:497:ASN:ND2	2:J:499:GLU:HB2	2.35	0.42
2:F:326:THR:O	2:F:326:THR:HG22	2.19	0.42
1:A:131:PHE:CD2	1:A:138:HIS:HB3	2.55	0.41
1:C:110:LYS:HA	1:C:111:PRO:HD2	1.93	0.41
1:G:3:GLU:OE2	1:G:3:GLU:HA	2.20	0.41
1:I:165:GLN:HE21	1:I:165:GLN:N	2.06	0.41
1:E:160:LEU:HD23	1:E:160:LEU:HA	1.89	0.41
2:H:392:VAL:HG21	2:H:527:LEU:HD12	2.02	0.41
2:H:451:ASN:HD22	2:H:490:PRO:HG2	1.85	0.41
1:I:160:LEU:HA	1:I:160:LEU:HD23	1.81	0.41
1:I:171:ILE:HD13	1:I:171:ILE:HG21	1.74	0.41
1:K:160:LEU:HD23	1:K:160:LEU:HA	1.83	0.41
1:E:15:PRO:CD	4:F:2550:DHB:C2	2.93	0.41
2:F:307:ARG:HA	2:F:307:ARG:HD3	1.85	0.41
2:F:318:LYS:NZ	2:F:318:LYS:CD	2.70	0.41
2:H:356:PHE:CE1	2:H:428:ARG:HD3	2.54	0.41
2:D:479:TYR:CZ	2:D:492:VAL:HG22	2.55	0.41
2:F:497:ASN:HD22	2:F:497:ASN:C	2.23	0.41
1:I:128:ILE:HD13	1:I:128:ILE:HG21	1.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:9:PRO:HD2	2:D:504:LEU:HD21	2.01	0.41
1:C:131:PHE:CE2	1:C:138:HIS:HB3	2.55	0.41
1:I:123:ALA:HB3	1:I:144:TYR:HE2	1.85	0.41
1:A:28:ASN:ND2	5:A:714:HOH:O	2.54	0.41
1:E:24:GLU:O	1:E:27:GLY:N	2.39	0.41
1:G:16:TYR:HE1	2:H:412:ASN:HB2	1.86	0.41
2:J:328:ILE:HD12	2:L:335:ALA:HB2	2.03	0.41
1:A:15:PRO:CD	4:B:550:DHB:C1	2.99	0.41
1:G:31:ARG:NH1	2:H:428:ARG:HG2	2.36	0.41
1:A:168:GLU:HA	1:A:171:ILE:HD12	2.02	0.41
2:B:307:ARG:HG2	2:B:533:THR:HG22	2.03	0.41
2:B:505:ILE:HD13	2:B:505:ILE:HG21	1.77	0.41
2:D:324:TYR:OH	4:D:1550:DHB:O1	2.26	0.41
1:K:165:GLN:H	1:K:165:GLN:HE21	1.68	0.41
2:L:361:HIS:CD2	2:L:361:HIS:N	2.81	0.41
1:E:190:GLN:HG3	2:F:333:ARG:HG2	2.03	0.40
2:H:417:ALA:HB1	5:H:3682:HOH:O	2.21	0.40
2:L:519:LEU:HD23	2:L:519:LEU:HA	1.89	0.40
2:B:335:ALA:HB2	2:F:328:ILE:HD12	2.03	0.40
1:C:18:HIS:CG	5:C:1648:HOH:O	2.72	0.40
1:E:17:VAL:CG1	1:E:18:HIS:N	2.85	0.40
1:E:143:LEU:HD23	1:E:143:LEU:C	2.42	0.40
1:I:23:LEU:CD1	1:I:23:LEU:N	2.84	0.40
1:I:26:ALA:O	2:J:411:LYS:NZ	2.54	0.40
1:K:31:ARG:HH12	2:L:428:ARG:HG2	1.83	0.40
2:L:356:PHE:HD1	2:L:428:ARG:HD3	1.85	0.40
2:B:326:THR:HG22	2:B:326:THR:O	2.21	0.40
2:F:411:LYS:HE2	2:F:411:LYS:HB2	1.95	0.40
2:J:522:ARG:HA	2:J:522:ARG:HD2	1.93	0.40
1:K:25:ALA:HB1	1:K:98:THR:HG21	2.03	0.40
1:A:129:SER:HA	1:A:139:LEU:O	2.22	0.40
2:L:429:CME:SG	2:L:437:TYR:HB2	2.61	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	198/200 (99%)	188 (95%)	10 (5%)	0	100	100
1	C	198/200 (99%)	189 (96%)	9 (4%)	0	100	100
1	E	198/200 (99%)	192 (97%)	6 (3%)	0	100	100
1	G	198/200 (99%)	190 (96%)	8 (4%)	0	100	100
1	I	198/200 (99%)	191 (96%)	6 (3%)	1 (0%)	29	19
1	K	198/200 (99%)	184 (93%)	14 (7%)	0	100	100
2	B	235/238 (99%)	227 (97%)	7 (3%)	1 (0%)	34	25
2	D	235/238 (99%)	227 (97%)	7 (3%)	1 (0%)	34	25
2	F	235/238 (99%)	227 (97%)	7 (3%)	1 (0%)	34	25
2	H	235/238 (99%)	227 (97%)	7 (3%)	1 (0%)	34	25
2	J	235/238 (99%)	226 (96%)	8 (3%)	1 (0%)	34	25
2	L	235/238 (99%)	226 (96%)	8 (3%)	1 (0%)	34	25
All	All	2598/2628 (99%)	2494 (96%)	97 (4%)	7 (0%)	41	32

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	368	ASN
2	D	368	ASN
2	F	368	ASN
2	J	368	ASN
2	L	368	ASN
2	H	535	PHE
1	I	132	ALA

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	162/163 (99%)	154 (95%)	8 (5%)	25 17
1	C	162/163 (99%)	149 (92%)	13 (8%)	12 5
1	E	162/163 (99%)	154 (95%)	8 (5%)	25 17
1	G	162/163 (99%)	153 (94%)	9 (6%)	21 13
1	I	162/163 (99%)	155 (96%)	7 (4%)	29 22
1	K	162/163 (99%)	154 (95%)	8 (5%)	25 17
2	B	199/201 (99%)	189 (95%)	10 (5%)	24 16
2	D	199/201 (99%)	187 (94%)	12 (6%)	19 11
2	F	199/201 (99%)	188 (94%)	11 (6%)	21 13
2	H	199/201 (99%)	186 (94%)	13 (6%)	17 9
2	J	199/201 (99%)	188 (94%)	11 (6%)	21 13
2	L	199/201 (99%)	188 (94%)	11 (6%)	21 13
All	All	2166/2184 (99%)	2045 (94%)	121 (6%)	21 13

All (121) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	38	ARG
1	A	52	LEU
1	A	91	SER
1	A	94	ARG
1	A	133	ARG
1	A	165	GLN
1	A	184	ARG
2	B	306	SER
2	B	364	LEU
2	B	372	LEU
2	B	395	THR
2	B	411	LYS
2	B	428	ARG
2	B	497	ASN
2	B	503	GLN
2	B	507	LYS
2	B	534	HIS
1	C	4	LEU
1	C	19	ILE
1	C	32	ASP
1	C	38	ARG

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Mol	Chain	Res	Type
1	C	42	PRO
1	C	52	LEU
1	C	94	ARG
1	C	106	LEU
1	C	133	ARG
1	C	158	LEU
1	C	165	GLN
1	C	178	ASP
1	C	184	ARG
2	D	364	LEU
2	D	372	LEU
2	D	393	PRO
2	D	395	THR
2	D	411	LYS
2	D	428	ARG
2	D	442	ILE
2	D	449	TRP
2	D	473	LYS
2	D	497	ASN
2	D	507	LYS
2	D	534	HIS
1	E	4	LEU
1	E	52	LEU
1	E	124	PRO
1	E	133	ARG
1	E	150	GLN
1	E	158	LEU
1	E	165	GLN
1	E	192	GLU
2	F	372	LEU
2	F	395	THR
2	F	399	MET
2	F	411	LYS
2	F	416	LEU
2	F	428	ARG
2	F	497	ASN
2	F	507	LYS
2	F	522	ARG
2	F	534	HIS
2	F	538	CYS
1	G	4	LEU
1	G	19	ILE

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Mol	Chain	Res	Type
1	G	38	ARG
1	G	52	LEU
1	G	94	ARG
1	G	154	LYS
1	G	158	LEU
1	G	165	GLN
1	G	184	ARG
2	H	352	SER
2	H	364	LEU
2	H	372	LEU
2	H	395	THR
2	H	399	MET
2	H	411	LYS
2	H	428	ARG
2	H	434	ASP
2	H	497	ASN
2	H	499	GLU
2	H	507	LYS
2	H	534	HIS
2	H	538	CYS
1	I	4	LEU
1	I	19	ILE
1	I	42	PRO
1	I	52	LEU
1	I	133	ARG
1	I	165	GLN
1	I	184	ARG
2	J	364	LEU
2	J	372	LEU
2	J	395	THR
2	J	399	MET
2	J	411	LYS
2	J	428	ARG
2	J	434	ASP
2	J	478	LEU
2	J	497	ASN
2	J	507	LYS
2	J	534	HIS
1	K	4	LEU
1	K	19	ILE
1	K	42	PRO
1	K	52	LEU

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Mol	Chain	Res	Type
1	K	94	ARG
1	K	133	ARG
1	K	165	GLN
1	K	184	ARG
2	L	306	SER
2	L	364	LEU
2	L	372	LEU
2	L	393	PRO
2	L	395	THR
2	L	411	LYS
2	L	428	ARG
2	L	497	ASN
2	L	507	LYS
2	L	534	HIS
2	L	538	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) 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
2	D	368	ASN
2	D	412	ASN
2	D	422	ASN
2	D	497	ASN
2	D	503	GLN
1	E	165	GLN
2	F	361	HIS
2	F	368	ASN
2	F	422	ASN
2	F	497	ASN
2	F	503	GLN
1	G	165	GLN
2	H	361	HIS

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Mol	Chain	Res	Type
2	H	422	ASN
2	H	497	ASN
2	H	503	GLN
1	I	163	GLN
1	I	165	GLN
2	J	361	HIS
2	J	368	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	422	ASN
2	L	497	ASN
2	L	503	GLN
2	L	530	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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	3.39	3 (37%)	5,9,11	2.95	3 (60%)
2	CME	H	429	2	8,9,10	3.57	4 (50%)	5,9,11	2.91	5 (100%)
2	CME	J	429	2	8,9,10	2.66	2 (25%)	5,9,11	1.73	2 (40%)
2	CME	D	429	2	8,9,10	2.80	3 (37%)	5,9,11	2.56	3 (60%)
2	CME	F	429	2	8,9,10	3.19	3 (37%)	5,9,11	1.82	2 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	CME	L	429	2	8,9,10	2.85	3 (37%)	5,9,11	2.98	3 (60%)

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	-	3/5/8/10	-
2	CME	H	429	2	-	3/5/8/10	-
2	CME	J	429	2	-	3/5/8/10	-
2	CME	D	429	2	-	3/5/8/10	-
2	CME	F	429	2	-	3/5/8/10	-
2	CME	L	429	2	-	3/5/8/10	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	429	CME	CB-SG	-7.93	1.56	1.81
2	F	429	CME	CB-SG	-7.17	1.58	1.81
2	H	429	CME	CB-SG	-6.92	1.59	1.81
2	D	429	CME	CB-SG	-6.49	1.60	1.81
2	J	429	CME	CB-SG	-6.44	1.60	1.81
2	L	429	CME	CB-SG	-6.13	1.61	1.81
2	H	429	CME	CE-CZ	5.29	1.86	1.50
2	F	429	CME	CE-CZ	4.09	1.78	1.50
2	H	429	CME	CE-SD	3.88	1.98	1.82
2	B	429	CME	CE-CZ	3.86	1.76	1.50
2	L	429	CME	CE-SD	3.80	1.98	1.82
2	J	429	CME	CE-CZ	3.33	1.73	1.50
2	B	429	CME	CE-SD	3.12	1.95	1.82
2	D	429	CME	CE-CZ	3.01	1.71	1.50
2	F	429	CME	CE-SD	2.83	1.94	1.82
2	H	429	CME	O-C	2.58	1.30	1.19
2	D	429	CME	CE-SD	2.49	1.92	1.82
2	L	429	CME	CA-N	-2.24	1.41	1.48

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	429	CME	CZ-CE-SD	-4.91	96.32	113.37
2	L	429	CME	CB-SG-SD	-4.30	92.68	103.82
2	H	429	CME	CB-SG-SD	-4.07	93.29	103.82
2	D	429	CME	CE-SD-SG	3.31	118.72	103.45
2	L	429	CME	CZ-CE-SD	-3.23	102.15	113.37
2	L	429	CME	CE-SD-SG	3.22	118.30	103.45
2	H	429	CME	CZ-CE-SD	-3.06	102.74	113.37
2	B	429	CME	OH-CZ-CE	3.06	122.91	110.83
2	B	429	CME	CE-SD-SG	2.81	116.41	103.45
2	D	429	CME	CZ-CE-SD	-2.79	103.69	113.37
2	J	429	CME	OH-CZ-CE	2.72	121.56	110.83
2	F	429	CME	CE-SD-SG	2.67	115.73	103.45
2	D	429	CME	OH-CZ-CE	2.57	120.98	110.83
2	H	429	CME	CE-SD-SG	2.43	114.64	103.45
2	H	429	CME	CA-CB-SG	2.40	124.78	114.55
2	F	429	CME	OH-CZ-CE	2.37	120.19	110.83
2	H	429	CME	OH-CZ-CE	2.18	119.44	110.83
2	J	429	CME	CE-SD-SG	2.04	112.86	103.45

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	429	CME	N-CA-CB-SG
2	H	429	CME	N-CA-CB-SG
2	L	429	CME	N-CA-CB-SG
2	B	429	CME	SD-CE-CZ-OH
2	D	429	CME	SD-CE-CZ-OH
2	F	429	CME	SD-CE-CZ-OH
2	H	429	CME	SD-CE-CZ-OH
2	J	429	CME	SD-CE-CZ-OH
2	L	429	CME	SD-CE-CZ-OH
2	D	429	CME	N-CA-CB-SG
2	F	429	CME	N-CA-CB-SG
2	J	429	CME	N-CA-CB-SG
2	B	429	CME	CZ-CE-SD-SG
2	H	429	CME	CZ-CE-SD-SG
2	L	429	CME	CZ-CE-SD-SG
2	J	429	CME	CE-SD-SG-CB
2	D	429	CME	CZ-CE-SD-SG
2	F	429	CME	CZ-CE-SD-SG

There are no ring outliers.

6 monomers are involved in 10 short contacts:

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

5.5 Carbohydrates (i)

There are no monosaccharides 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	L	5550	3	9,11,11	0.88	1 (11%)	12,15,15	0.54	0
4	DHB	J	4550	3	9,11,11	0.91	0	12,15,15	0.44	0
4	DHB	F	2550	3	9,11,11	1.22	2 (22%)	12,15,15	0.54	0
4	DHB	B	550	3	9,11,11	1.52	2 (22%)	12,15,15	0.69	0
4	DHB	H	3550	3	9,11,11	1.88	4 (44%)	12,15,15	0.78	0
4	DHB	D	1550	3	9,11,11	1.33	2 (22%)	12,15,15	0.57	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	L	5550	3	-	0/0/4/4	0/1/1/1
4	DHB	J	4550	3	-	0/0/4/4	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	DHB	F	2550	3	-	0/0/4/4	0/1/1/1
4	DHB	B	550	3	-	0/0/4/4	0/1/1/1
4	DHB	H	3550	3	-	0/0/4/4	0/1/1/1
4	DHB	D	1550	3	-	0/0/4/4	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1550	DHB	C1-C	-2.98	1.44	1.47
4	B	550	DHB	C4-C3	-2.79	1.35	1.40
4	H	3550	DHB	C2-C3	-2.73	1.35	1.38
4	F	2550	DHB	C4-C3	-2.53	1.36	1.40
4	H	3550	DHB	C5-C4	-2.53	1.35	1.39
4	D	1550	DHB	C4-C3	-2.30	1.36	1.40
4	B	550	DHB	C1-C	-2.24	1.45	1.47
4	H	3550	DHB	C1-C	-2.19	1.45	1.47
4	L	5550	DHB	C1-C	-2.18	1.45	1.47
4	H	3550	DHB	C4-C3	-2.07	1.36	1.40
4	F	2550	DHB	C1-C	-2.01	1.45	1.47

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 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	5550	DHB	4	0
4	J	4550	DHB	3	0
4	F	2550	DHB	8	0
4	B	550	DHB	4	0
4	H	3550	DHB	5	0
4	D	1550	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%)	-0.43	6 (3%)	50	53	6, 18, 47, 61	0
1	C	200/200 (100%)	-0.40	5 (2%)	57	60	7, 19, 45, 62	0
1	E	200/200 (100%)	-0.35	8 (4%)	38	40	7, 20, 48, 61	0
1	G	200/200 (100%)	-0.33	9 (4%)	33	34	7, 20, 49, 62	0
1	I	200/200 (100%)	-0.27	11 (5%)	25	26	8, 21, 49, 63	0
1	K	200/200 (100%)	-0.17	12 (6%)	21	22	9, 23, 49, 62	0
2	B	237/238 (99%)	-0.61	8 (3%)	45	47	7, 13, 38, 58	0
2	D	237/238 (99%)	-0.60	7 (2%)	50	53	6, 13, 39, 60	0
2	F	237/238 (99%)	-0.65	8 (3%)	45	47	5, 14, 38, 58	0
2	H	237/238 (99%)	-0.64	6 (2%)	57	60	7, 14, 39, 54	0
2	J	237/238 (99%)	-0.64	6 (2%)	57	60	7, 15, 39, 59	0
2	L	237/238 (99%)	-0.65	6 (2%)	57	60	9, 15, 39, 59	0
All	All	2622/2628 (99%)	-0.49	92 (3%)	44	46	5, 17, 46, 63	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	99	PHE	6.0
2	D	369	ASN	5.6
2	L	301	PRO	5.1
1	C	100	ASP	5.1
1	K	178	ASP	5.0
1	K	99	PHE	5.0
2	J	369	ASN	5.0
2	J	370	GLY	4.9
1	K	179	GLY	4.8
2	B	370	GLY	4.7
2	D	368	ASN	4.7

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Mol	Chain	Res	Type	RSRZ
1	G	101	ALA	4.6
2	J	368	ASN	4.4
1	C	99	PHE	4.2
1	G	99	PHE	4.2
2	L	370	GLY	4.2
2	L	369	ASN	4.1
1	I	178	ASP	4.1
1	I	179	GLY	4.1
1	K	177	VAL	4.0
1	A	99	PHE	4.0
2	D	301	PRO	4.0
1	A	178	ASP	3.9
1	G	100	ASP	3.9
2	F	370	GLY	3.8
1	E	99	PHE	3.8
1	K	101	ALA	3.8
1	K	100	ASP	3.8
2	H	301	PRO	3.7
2	B	369	ASN	3.7
2	D	370	GLY	3.6
2	H	414	ARG	3.5
1	G	178	ASP	3.4
1	E	178	ASP	3.4
1	G	177	VAL	3.3
1	I	100	ASP	3.3
1	I	177	VAL	3.3
1	C	101	ALA	3.3
2	F	369	ASN	3.3
2	F	301	PRO	3.2
1	E	176	GLU	3.2
1	K	176	GLU	3.2
2	B	414	ARG	3.2
2	L	368	ASN	3.1
1	G	27	GLY	3.0
1	A	100	ASP	3.0
1	E	100	ASP	3.0
1	G	176	GLU	3.0
2	D	537	ASN	2.9
2	L	537	ASN	2.9
2	B	538	CYS	2.9
1	I	101	ALA	2.8
1	K	43	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
2	J	301	PRO	2.8
1	I	42	PRO	2.7
2	J	537	ASN	2.7
2	B	368	ASN	2.7
1	I	43	ASP	2.6
2	H	370	GLY	2.6
2	J	414	ARG	2.6
2	D	414	ARG	2.6
1	G	179	GLY	2.5
1	I	176	GLU	2.5
1	A	179	GLY	2.5
1	K	192	GLU	2.5
2	B	537	ASN	2.5
2	B	301	PRO	2.5
2	H	411	LYS	2.5
2	F	414	ARG	2.5
1	K	150	GLN	2.4
2	F	368	ASN	2.4
1	A	43	ASP	2.4
1	E	179	GLY	2.4
2	L	414	ARG	2.4
1	A	42	PRO	2.4
2	H	537	ASN	2.4
1	E	86	GLU	2.4
2	F	537	ASN	2.3
1	E	101	ALA	2.3
2	B	305	ASN	2.3
2	H	538	CYS	2.3
1	C	32	ASP	2.3
1	I	32	ASP	2.3
1	I	24	GLU	2.2
1	K	42	PRO	2.2
2	D	538	CYS	2.2
1	C	42	PRO	2.1
1	E	177	VAL	2.1
2	F	411	LYS	2.1
1	G	24	GLU	2.1
1	K	44	ALA	2.1
2	F	538	CYS	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. 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	B-factors(Å^2)	Q<0.9
2	CME	D	429	10/11	0.92	0.12	17,25,51,51	0
2	CME	F	429	10/11	0.93	0.12	16,23,49,50	0
2	CME	H	429	10/11	0.93	0.12	14,23,49,49	0
2	CME	L	429	10/11	0.94	0.10	19,27,49,50	0
2	CME	J	429	10/11	0.95	0.10	20,26,50,51	0
2	CME	B	429	10/11	0.95	0.11	14,24,46,47	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{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	B-factors(Å^2)	Q<0.9
3	FE	H	3600	1/1	0.68	0.09	82,82,82,82	0
3	FE	L	5600	1/1	0.70	0.07	75,75,75,75	0
3	FE	F	2600	1/1	0.79	0.07	77,77,77,77	0
4	DHB	L	5550	11/11	0.79	0.19	54,56,58,60	0
4	DHB	B	550	11/11	0.80	0.19	46,49,50,51	0
3	FE	B	600	1/1	0.81	0.08	83,83,83,83	0
4	DHB	J	4550	11/11	0.82	0.18	50,51,52,53	0
4	DHB	F	2550	11/11	0.82	0.21	55,57,59,60	0
4	DHB	D	1550	11/11	0.84	0.19	51,52,55,55	0
3	FE	D	1600	1/1	0.89	0.06	69,69,69,69	0
4	DHB	H	3550	11/11	0.89	0.18	54,55,57,57	0
3	FE	J	4600	1/1	0.91	0.07	80,80,80,80	0

6.5 Other polymers (i)

There are no such residues in this entry.