Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2021 – 09:59 PM EST

PDB ID	:	1CYC
Title	:	THE CRYSTAL STRUCTURE OF BONITO (KATSUO) FERROCYTOCHROME C AT 2.3 ANGSTROMS RESOLUTION. II. STRUCTURE AND FUNCTION
Authors	:	Tanaka, N.; Yamane, T.; Tsukihara, T.; Ashida, T.; Kakudo, M.
Deposited on	:	1976-08-01
Resolution	:	2.30 Å(reported)

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

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

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

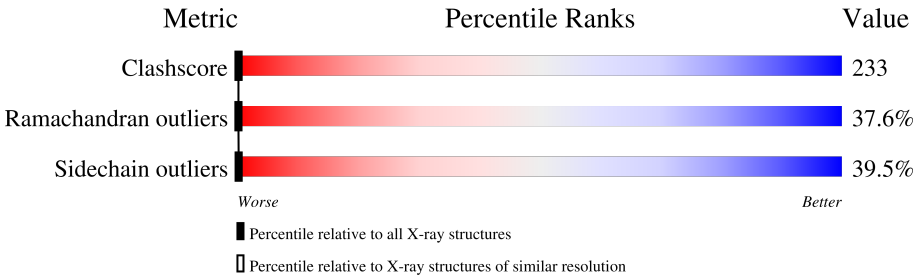
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.17.1

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 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	103	. 32% 65%
1	B	103	. 32% 65%

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	HEC	A	104	-	-	X	-
2	HEC	B	104	-	-	X	-

2 Entry composition

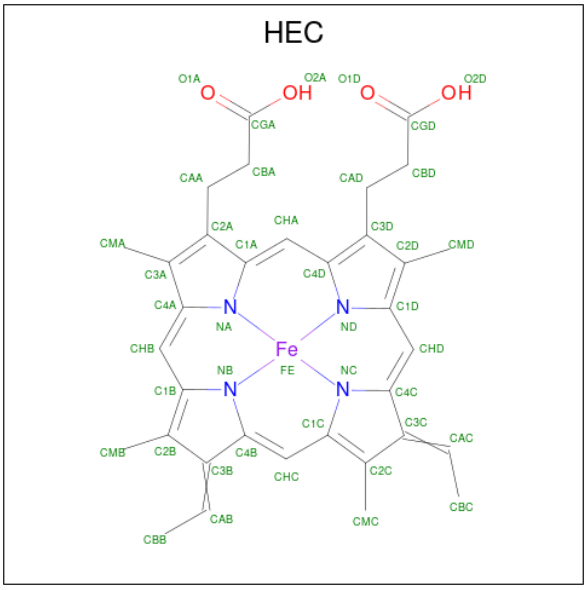
There are 3 unique types of molecules in this entry. The entry contains 1677 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 FERROCYTOCHROME C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	103	Total	C	N	O	S	0	0	0
			795	505	139	147	4			
1	B	103	Total	C	N	O	S	0	0	0
			795	505	139	147	4			

- Molecule 2 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O 1 1	0	0

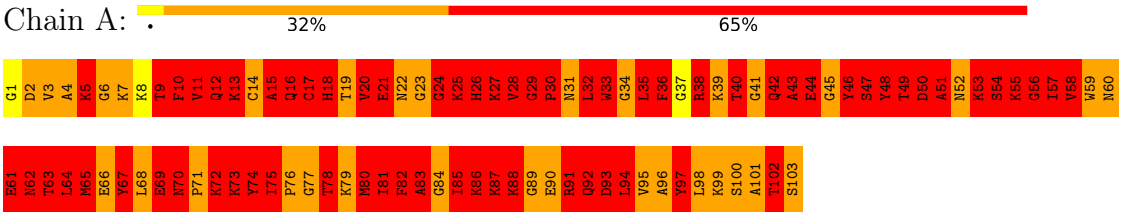
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

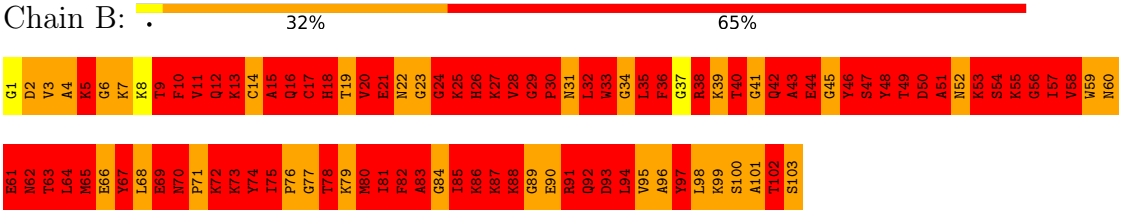
• Molecule 1: FERROCYTOCHROME C

Chain A:



• Molecule 1: FERROCYTOCHROME C

Chain B:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	57.68Å 84.58Å 37.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1677	wwPDB-VP
Average B, all atoms (Å^2)	0.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

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

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	7.94	366/811 (45.1%)	6.18	322/1084 (29.7%)
1	B	7.94	366/811 (45.1%)	6.18	322/1084 (29.7%)
All	All	7.94	732/1622 (45.1%)	6.18	644/2168 (29.7%)

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	2	35
1	B	2	35
All	All	4	70

All (732) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	3	VAL	CA-CB	60.22	2.81	1.54
1	B	3	VAL	CA-CB	60.22	2.81	1.54
1	A	44	GLU	CG-CD	37.82	2.08	1.51
1	B	44	GLU	CG-CD	37.82	2.08	1.51
1	A	46	TYR	CG-CD1	-37.48	0.90	1.39
1	B	46	TYR	CG-CD1	-37.48	0.90	1.39
1	A	10	PHE	CG-CD2	-30.47	0.93	1.38
1	B	10	PHE	CG-CD2	-30.47	0.93	1.38
1	A	44	GLU	CB-CG	30.30	2.09	1.52
1	B	44	GLU	CB-CG	30.30	2.09	1.52
1	A	46	TYR	CE2-CZ	-28.09	1.02	1.38
1	B	46	TYR	CE2-CZ	-28.09	1.02	1.38
1	A	30	PRO	N-CD	-27.34	1.09	1.47
1	B	30	PRO	N-CD	-27.34	1.09	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	61	GLU	CD-OE2	26.47	1.54	1.25
1	A	90	GLU	CD-OE2	26.47	1.54	1.25
1	B	61	GLU	CD-OE2	26.47	1.54	1.25
1	B	90	GLU	CD-OE2	26.47	1.54	1.25
1	A	24	GLY	N-CA	25.53	1.84	1.46
1	B	24	GLY	N-CA	25.53	1.84	1.46
1	A	59	TRP	CD2-CE2	-24.98	1.11	1.41
1	B	59	TRP	CD2-CE2	-24.98	1.11	1.41
1	A	21	GLU	CD-OE1	24.59	1.52	1.25
1	A	69	GLU	CD-OE1	24.59	1.52	1.25
1	B	21	GLU	CD-OE1	24.59	1.52	1.25
1	B	69	GLU	CD-OE1	24.59	1.52	1.25
1	A	21	GLU	CD-OE2	24.23	1.52	1.25
1	B	21	GLU	CD-OE2	24.23	1.52	1.25
1	A	33	TRP	CE2-CZ2	-23.23	1.00	1.39
1	B	33	TRP	CE2-CZ2	-23.23	1.00	1.39
1	A	38	ARG	CZ-NH1	-22.37	1.03	1.33
1	B	38	ARG	CZ-NH1	-22.37	1.03	1.33
1	A	73	LYS	CD-CE	21.45	2.04	1.51
1	B	73	LYS	CD-CE	21.45	2.04	1.51
1	A	90	GLU	CD-OE1	21.23	1.49	1.25
1	B	90	GLU	CD-OE1	21.23	1.49	1.25
1	A	91	ARG	CZ-NH1	21.08	1.60	1.33
1	B	91	ARG	CZ-NH1	21.08	1.60	1.33
1	A	47	SER	CB-OG	20.60	1.69	1.42
1	B	47	SER	CB-OG	20.60	1.69	1.42
1	A	67	TYR	CE1-CZ	-20.49	1.11	1.38
1	B	67	TYR	CE1-CZ	-20.49	1.11	1.38
1	A	44	GLU	CD-OE2	20.25	1.48	1.25
1	B	44	GLU	CD-OE2	20.25	1.48	1.25
1	A	54	SER	CA-CB	-20.23	1.22	1.52
1	B	54	SER	CA-CB	-20.23	1.22	1.52
1	A	91	ARG	NE-CZ	19.54	1.58	1.33
1	B	91	ARG	NE-CZ	19.54	1.58	1.33
1	A	81	ILE	C-O	19.46	1.60	1.23
1	B	81	ILE	C-O	19.46	1.60	1.23
1	A	82	PHE	CG-CD2	-19.45	1.09	1.38
1	B	82	PHE	CG-CD2	-19.45	1.09	1.38
1	A	92	GLN	CD-OE1	19.03	1.65	1.24
1	B	92	GLN	CD-OE1	19.03	1.65	1.24
1	A	19	THR	CB-OG1	-18.97	1.05	1.43
1	B	19	THR	CB-OG1	-18.97	1.05	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	83	ALA	CA-CB	18.61	1.91	1.52
1	B	83	ALA	CA-CB	18.61	1.91	1.52
1	A	63	THR	CB-OG1	-18.60	1.06	1.43
1	B	63	THR	CB-OG1	-18.60	1.06	1.43
1	A	12	GLN	CG-CD	18.59	1.93	1.51
1	B	12	GLN	CG-CD	18.59	1.93	1.51
1	A	33	TRP	CZ3-CH2	-18.48	1.10	1.40
1	B	33	TRP	CZ3-CH2	-18.48	1.10	1.40
1	A	48	TYR	CG-CD2	-18.39	1.15	1.39
1	B	48	TYR	CG-CD2	-18.39	1.15	1.39
1	A	45	GLY	C-O	18.15	1.52	1.23
1	B	45	GLY	C-O	18.15	1.52	1.23
1	A	12	GLN	CD-OE1	17.77	1.63	1.24
1	B	12	GLN	CD-OE1	17.77	1.63	1.24
1	A	46	TYR	CZ-OH	-17.07	1.08	1.37
1	B	46	TYR	CZ-OH	-17.07	1.08	1.37
1	A	28	VAL	CA-CB	-16.79	1.19	1.54
1	B	28	VAL	CA-CB	-16.79	1.19	1.54
1	A	71	PRO	N-CA	-16.53	1.19	1.47
1	B	71	PRO	N-CA	-16.53	1.19	1.47
1	A	64	LEU	CA-CB	16.43	1.91	1.53
1	B	64	LEU	CA-CB	16.43	1.91	1.53
1	A	64	LEU	C-O	-15.95	0.93	1.23
1	B	64	LEU	C-O	-15.95	0.93	1.23
1	A	26	HIS	CB-CG	15.95	1.78	1.50
1	B	26	HIS	CB-CG	15.95	1.78	1.50
1	A	2	ASP	CG-OD1	15.90	1.61	1.25
1	B	2	ASP	CG-OD1	15.90	1.61	1.25
1	A	2	ASP	CG-OD2	15.21	1.60	1.25
1	B	2	ASP	CG-OD2	15.21	1.60	1.25
1	A	92	GLN	N-CA	15.03	1.76	1.46
1	B	92	GLN	N-CA	15.03	1.76	1.46
1	A	56	GLY	N-CA	15.00	1.68	1.46
1	B	56	GLY	N-CA	15.00	1.68	1.46
1	A	66	GLU	CD-OE1	14.76	1.41	1.25
1	B	66	GLU	CD-OE1	14.76	1.41	1.25
1	A	61	GLU	CD-OE1	14.25	1.41	1.25
1	B	61	GLU	CD-OE1	14.25	1.41	1.25
1	A	48	TYR	CE1-CZ	-14.15	1.20	1.38
1	B	48	TYR	CE1-CZ	-14.15	1.20	1.38
1	A	88	LYS	CD-CE	-14.13	1.16	1.51
1	B	88	LYS	CD-CE	-14.13	1.16	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	10	PHE	CD2-CE2	-14.12	1.11	1.39
1	B	10	PHE	CD2-CE2	-14.12	1.11	1.39
1	A	98	LEU	N-CA	13.66	1.73	1.46
1	B	98	LEU	N-CA	13.66	1.73	1.46
1	A	40	THR	C-N	-13.45	1.08	1.33
1	B	40	THR	C-N	-13.45	1.08	1.33
1	A	20	VAL	CB-CG1	-13.40	1.24	1.52
1	B	20	VAL	CB-CG1	-13.40	1.24	1.52
1	A	30	PRO	CA-CB	-13.24	1.27	1.53
1	A	93	ASP	CG-OD1	13.24	1.55	1.25
1	B	30	PRO	CA-CB	-13.24	1.27	1.53
1	B	93	ASP	CG-OD1	13.24	1.55	1.25
1	A	103	SER	C-O	13.22	1.48	1.23
1	B	103	SER	C-O	13.22	1.48	1.23
1	A	101	ALA	N-CA	13.20	1.72	1.46
1	B	101	ALA	N-CA	13.20	1.72	1.46
1	A	62	ASN	CG-OD1	13.07	1.52	1.24
1	B	62	ASN	CG-OD1	13.07	1.52	1.24
1	A	57	ILE	CA-CB	-12.90	1.25	1.54
1	B	57	ILE	CA-CB	-12.90	1.25	1.54
1	A	70	ASN	CG-OD1	12.83	1.52	1.24
1	B	70	ASN	CG-OD1	12.83	1.52	1.24
1	A	16	GLN	N-CA	12.80	1.72	1.46
1	B	16	GLN	N-CA	12.80	1.72	1.46
1	A	33	TRP	CZ2-CH2	-12.64	1.13	1.37
1	B	33	TRP	CZ2-CH2	-12.64	1.13	1.37
1	A	32	LEU	C-N	-12.50	1.05	1.34
1	B	32	LEU	C-N	-12.50	1.05	1.34
1	A	89	GLY	N-CA	12.46	1.64	1.46
1	B	89	GLY	N-CA	12.46	1.64	1.46
1	A	82	PHE	CE2-CZ	-12.28	1.14	1.37
1	B	82	PHE	CE2-CZ	-12.28	1.14	1.37
1	A	13	LYS	C-O	-12.15	1.00	1.23
1	B	13	LYS	C-O	-12.15	1.00	1.23
1	A	62	ASN	N-CA	12.10	1.70	1.46
1	B	62	ASN	N-CA	12.10	1.70	1.46
1	A	43	ALA	N-CA	12.04	1.70	1.46
1	B	43	ALA	N-CA	12.04	1.70	1.46
1	A	37	GLY	CA-C	-11.94	1.32	1.51
1	B	37	GLY	CA-C	-11.94	1.32	1.51
1	A	50	ASP	CG-OD1	11.89	1.52	1.25
1	B	50	ASP	CG-OD1	11.89	1.52	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	33	TRP	N-CA	11.87	1.70	1.46
1	A	91	ARG	N-CA	11.87	1.70	1.46
1	B	33	TRP	N-CA	11.87	1.70	1.46
1	B	91	ARG	N-CA	11.87	1.70	1.46
1	A	82	PHE	N-CA	11.81	1.70	1.46
1	B	82	PHE	N-CA	11.81	1.70	1.46
1	A	22	ASN	C-N	-11.74	1.11	1.33
1	B	22	ASN	C-N	-11.74	1.11	1.33
1	A	49	THR	CA-C	-11.67	1.22	1.52
1	B	49	THR	CA-C	-11.67	1.22	1.52
1	A	42	GLN	CG-CD	-11.66	1.24	1.51
1	B	42	GLN	CG-CD	-11.66	1.24	1.51
1	A	59	TRP	CZ3-CH2	-11.61	1.21	1.40
1	B	59	TRP	CZ3-CH2	-11.61	1.21	1.40
1	A	42	GLN	CD-NE2	11.48	1.61	1.32
1	B	42	GLN	CD-NE2	11.48	1.61	1.32
1	A	59	TRP	N-CA	11.34	1.69	1.46
1	B	59	TRP	N-CA	11.34	1.69	1.46
1	A	36	PHE	CD2-CE2	-11.32	1.16	1.39
1	B	36	PHE	CD2-CE2	-11.32	1.16	1.39
1	A	50	ASP	C-O	11.22	1.44	1.23
1	B	50	ASP	C-O	11.22	1.44	1.23
1	A	59	TRP	C-N	-11.20	1.08	1.34
1	B	59	TRP	C-N	-11.20	1.08	1.34
1	A	32	LEU	N-CA	11.10	1.68	1.46
1	B	32	LEU	N-CA	11.10	1.68	1.46
1	A	100	SER	CA-CB	11.03	1.69	1.52
1	B	100	SER	CA-CB	11.03	1.69	1.52
1	A	31	ASN	CG-OD1	10.96	1.48	1.24
1	A	93	ASP	C-N	-10.96	1.08	1.34
1	B	31	ASN	CG-OD1	10.96	1.48	1.24
1	B	93	ASP	C-N	-10.96	1.08	1.34
1	A	67	TYR	CD1-CE1	-10.94	1.23	1.39
1	B	67	TYR	CD1-CE1	-10.94	1.23	1.39
1	A	100	SER	C-O	10.93	1.44	1.23
1	B	100	SER	C-O	10.93	1.44	1.23
1	A	86	LYS	C-N	-10.88	1.09	1.34
1	B	86	LYS	C-N	-10.88	1.09	1.34
1	A	18	HIS	N-CA	10.87	1.68	1.46
1	B	18	HIS	N-CA	10.87	1.68	1.46
1	A	53	LYS	CD-CE	10.82	1.78	1.51
1	B	53	LYS	CD-CE	10.82	1.78	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	33	TRP	CB-CG	-10.81	1.30	1.50
1	B	33	TRP	CB-CG	-10.81	1.30	1.50
1	A	52	ASN	CA-C	-10.80	1.24	1.52
1	B	52	ASN	CA-C	-10.80	1.24	1.52
1	A	16	GLN	CD-OE1	10.78	1.47	1.24
1	B	16	GLN	CD-OE1	10.78	1.47	1.24
1	A	60	ASN	CG-OD1	10.72	1.47	1.24
1	B	60	ASN	CG-OD1	10.72	1.47	1.24
1	A	50	ASP	CB-CG	-10.57	1.29	1.51
1	B	50	ASP	CB-CG	-10.57	1.29	1.51
1	A	30	PRO	C-N	10.55	1.58	1.34
1	B	30	PRO	C-N	10.55	1.58	1.34
1	A	42	GLN	CD-OE1	10.53	1.47	1.24
1	B	42	GLN	CD-OE1	10.53	1.47	1.24
1	A	86	LYS	CD-CE	10.42	1.77	1.51
1	B	86	LYS	CD-CE	10.42	1.77	1.51
1	A	23	GLY	N-CA	10.34	1.61	1.46
1	B	23	GLY	N-CA	10.34	1.61	1.46
1	A	101	ALA	CA-CB	-10.32	1.30	1.52
1	B	101	ALA	CA-CB	-10.32	1.30	1.52
1	A	7	LYS	N-CA	10.21	1.66	1.46
1	B	7	LYS	N-CA	10.21	1.66	1.46
1	A	8	LYS	C-O	-10.20	1.03	1.23
1	B	8	LYS	C-O	-10.20	1.03	1.23
1	A	41	GLY	C-O	-10.18	1.07	1.23
1	A	77	GLY	C-O	-10.18	1.07	1.23
1	B	41	GLY	C-O	-10.18	1.07	1.23
1	B	77	GLY	C-O	-10.18	1.07	1.23
1	A	67	TYR	CE2-CZ	-10.16	1.25	1.38
1	B	67	TYR	CE2-CZ	-10.16	1.25	1.38
1	A	46	TYR	N-CA	10.15	1.66	1.46
1	B	46	TYR	N-CA	10.15	1.66	1.46
1	A	3	VAL	CA-C	10.01	1.78	1.52
1	B	3	VAL	CA-C	10.01	1.78	1.52
1	A	33	TRP	CD2-CE2	-9.95	1.29	1.41
1	B	33	TRP	CD2-CE2	-9.95	1.29	1.41
1	A	53	LYS	N-CA	9.91	1.66	1.46
1	B	53	LYS	N-CA	9.91	1.66	1.46
1	A	73	LYS	CE-NZ	-9.80	1.24	1.49
1	B	73	LYS	CE-NZ	-9.80	1.24	1.49
1	A	61	GLU	CG-CD	-9.75	1.37	1.51
1	B	61	GLU	CG-CD	-9.75	1.37	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	33	TRP	CG-CD2	-9.75	1.27	1.43
1	B	33	TRP	CG-CD2	-9.75	1.27	1.43
1	A	57	ILE	C-N	9.68	1.56	1.34
1	B	57	ILE	C-N	9.68	1.56	1.34
1	A	71	PRO	CA-CB	-9.65	1.34	1.53
1	B	71	PRO	CA-CB	-9.65	1.34	1.53
1	A	17	CYS	CA-CB	9.64	1.75	1.53
1	B	17	CYS	CA-CB	9.64	1.75	1.53
1	A	51	ALA	C-O	-9.60	1.05	1.23
1	B	51	ALA	C-O	-9.60	1.05	1.23
1	A	44	GLU	CD-OE1	9.55	1.36	1.25
1	B	44	GLU	CD-OE1	9.55	1.36	1.25
1	A	82	PHE	CG-CD1	-9.47	1.24	1.38
1	B	82	PHE	CG-CD1	-9.47	1.24	1.38
1	A	32	LEU	C-O	9.46	1.41	1.23
1	B	32	LEU	C-O	9.46	1.41	1.23
1	A	67	TYR	CD2-CE2	-9.44	1.25	1.39
1	B	67	TYR	CD2-CE2	-9.44	1.25	1.39
1	A	61	GLU	N-CA	9.43	1.65	1.46
1	B	61	GLU	N-CA	9.43	1.65	1.46
1	A	74	TYR	CE2-CZ	-9.31	1.26	1.38
1	B	74	TYR	CE2-CZ	-9.31	1.26	1.38
1	A	48	TYR	CG-CD1	-9.29	1.27	1.39
1	B	48	TYR	CG-CD1	-9.29	1.27	1.39
1	A	30	PRO	CB-CG	-9.27	1.03	1.50
1	B	30	PRO	CB-CG	-9.27	1.03	1.50
1	A	54	SER	CB-OG	9.23	1.54	1.42
1	A	100	SER	CB-OG	9.23	1.54	1.42
1	B	54	SER	CB-OG	9.23	1.54	1.42
1	B	100	SER	CB-OG	9.23	1.54	1.42
1	A	102	THR	N-CA	9.19	1.64	1.46
1	B	102	THR	N-CA	9.19	1.64	1.46
1	A	48	TYR	CE2-CZ	-9.19	1.26	1.38
1	B	48	TYR	CE2-CZ	-9.19	1.26	1.38
1	A	93	ASP	CG-OD2	9.11	1.46	1.25
1	B	93	ASP	CG-OD2	9.11	1.46	1.25
1	A	82	PHE	C-N	-9.09	1.13	1.34
1	B	82	PHE	C-N	-9.09	1.13	1.34
1	A	55	LYS	C-N	-9.04	1.16	1.33
1	B	55	LYS	C-N	-9.04	1.16	1.33
1	A	29	GLY	C-N	9.02	1.51	1.34
1	B	29	GLY	C-N	9.02	1.51	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	29	GLY	N-CA	-8.97	1.32	1.46
1	B	29	GLY	N-CA	-8.97	1.32	1.46
1	A	77	GLY	CA-C	8.95	1.66	1.51
1	B	77	GLY	CA-C	8.95	1.66	1.51
1	A	16	GLN	CD-NE2	-8.95	1.10	1.32
1	A	21	GLU	N-CA	8.95	1.64	1.46
1	A	65	MET	N-CA	8.95	1.64	1.46
1	A	81	ILE	N-CA	8.95	1.64	1.46
1	B	16	GLN	CD-NE2	-8.95	1.10	1.32
1	B	21	GLU	N-CA	8.95	1.64	1.46
1	B	65	MET	N-CA	8.95	1.64	1.46
1	B	81	ILE	N-CA	8.95	1.64	1.46
1	A	66	GLU	C-N	-8.94	1.13	1.34
1	B	66	GLU	C-N	-8.94	1.13	1.34
1	A	46	TYR	C-N	-8.86	1.13	1.34
1	B	46	TYR	C-N	-8.86	1.13	1.34
1	A	98	LEU	CA-C	8.85	1.75	1.52
1	B	98	LEU	CA-C	8.85	1.75	1.52
1	A	59	TRP	CE2-CZ2	8.83	1.54	1.39
1	B	59	TRP	CE2-CZ2	8.83	1.54	1.39
1	A	12	GLN	N-CA	8.83	1.64	1.46
1	B	12	GLN	N-CA	8.83	1.64	1.46
1	A	24	GLY	C-O	8.82	1.37	1.23
1	B	24	GLY	C-O	8.82	1.37	1.23
1	A	26	HIS	CG-CD2	-8.79	1.20	1.35
1	B	26	HIS	CG-CD2	-8.79	1.20	1.35
1	A	89	GLY	C-N	-8.78	1.13	1.34
1	A	98	LEU	CB-CG	-8.78	1.27	1.52
1	B	89	GLY	C-N	-8.78	1.13	1.34
1	B	98	LEU	CB-CG	-8.78	1.27	1.52
1	A	62	ASN	CA-CB	-8.78	1.30	1.53
1	B	62	ASN	CA-CB	-8.78	1.30	1.53
1	A	59	TRP	CD2-CE3	-8.74	1.27	1.40
1	B	59	TRP	CD2-CE3	-8.74	1.27	1.40
1	A	49	THR	N-CA	8.71	1.63	1.46
1	B	49	THR	N-CA	8.71	1.63	1.46
1	A	82	PHE	CE1-CZ	-8.71	1.20	1.37
1	B	82	PHE	CE1-CZ	-8.71	1.20	1.37
1	A	55	LYS	CD-CE	8.65	1.72	1.51
1	B	55	LYS	CD-CE	8.65	1.72	1.51
1	A	7	LYS	C-O	8.64	1.39	1.23
1	B	7	LYS	C-O	8.64	1.39	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	50	ASP	CA-CB	-8.62	1.34	1.53
1	B	50	ASP	CA-CB	-8.62	1.34	1.53
1	A	64	LEU	CG-CD1	-8.61	1.20	1.51
1	B	64	LEU	CG-CD1	-8.61	1.20	1.51
1	A	52	ASN	C-O	8.56	1.39	1.23
1	B	52	ASN	C-O	8.56	1.39	1.23
1	A	47	SER	N-CA	8.53	1.63	1.46
1	A	60	ASN	N-CA	8.53	1.63	1.46
1	B	47	SER	N-CA	8.53	1.63	1.46
1	B	60	ASN	N-CA	8.53	1.63	1.46
1	A	95	VAL	CB-CG2	-8.51	1.34	1.52
1	B	95	VAL	CB-CG2	-8.51	1.34	1.52
1	A	65	MET	C-N	-8.48	1.14	1.34
1	A	69	GLU	C-N	-8.48	1.14	1.34
1	B	65	MET	C-N	-8.48	1.14	1.34
1	B	69	GLU	C-N	-8.48	1.14	1.34
1	A	78	THR	CA-C	-8.47	1.30	1.52
1	B	78	THR	CA-C	-8.47	1.30	1.52
1	A	97	TYR	CE2-CZ	8.45	1.49	1.38
1	B	97	TYR	CE2-CZ	8.45	1.49	1.38
1	A	61	GLU	CB-CG	-8.42	1.36	1.52
1	B	61	GLU	CB-CG	-8.42	1.36	1.52
1	A	40	THR	CB-OG1	8.35	1.59	1.43
1	B	40	THR	CB-OG1	8.35	1.59	1.43
1	A	14	CYS	N-CA	8.34	1.63	1.46
1	B	14	CYS	N-CA	8.34	1.63	1.46
1	A	58	VAL	CA-CB	-8.30	1.37	1.54
1	B	58	VAL	CA-CB	-8.30	1.37	1.54
1	A	86	LYS	CG-CD	8.22	1.80	1.52
1	B	86	LYS	CG-CD	8.22	1.80	1.52
1	A	100	SER	N-CA	8.22	1.62	1.46
1	B	100	SER	N-CA	8.22	1.62	1.46
1	A	49	THR	CA-CB	8.21	1.74	1.53
1	B	49	THR	CA-CB	8.21	1.74	1.53
1	A	55	LYS	CA-C	8.19	1.74	1.52
1	A	91	ARG	CZ-NH2	8.19	1.43	1.33
1	B	55	LYS	CA-C	8.19	1.74	1.52
1	B	91	ARG	CZ-NH2	8.19	1.43	1.33
1	A	60	ASN	C-N	-8.18	1.15	1.34
1	A	90	GLU	C-N	-8.18	1.15	1.34
1	B	60	ASN	C-N	-8.18	1.15	1.34
1	B	90	GLU	C-N	-8.18	1.15	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	68	LEU	CA-CB	-8.16	1.34	1.53
1	B	68	LEU	CA-CB	-8.16	1.34	1.53
1	A	103	SER	CB-OG	8.14	1.52	1.42
1	B	103	SER	CB-OG	8.14	1.52	1.42
1	A	74	TYR	CA-CB	8.13	1.71	1.53
1	B	74	TYR	CA-CB	8.13	1.71	1.53
1	A	77	GLY	C-N	8.11	1.52	1.34
1	B	77	GLY	C-N	8.11	1.52	1.34
1	A	79	LYS	CA-CB	-8.09	1.36	1.53
1	B	79	LYS	CA-CB	-8.09	1.36	1.53
1	A	7	LYS	CA-CB	8.02	1.71	1.53
1	B	7	LYS	CA-CB	8.02	1.71	1.53
1	A	19	THR	N-CA	7.97	1.62	1.46
1	B	19	THR	N-CA	7.97	1.62	1.46
1	A	14	CYS	CA-CB	7.97	1.71	1.53
1	A	102	THR	CA-C	7.97	1.73	1.52
1	B	14	CYS	CA-CB	7.97	1.71	1.53
1	B	102	THR	CA-C	7.97	1.73	1.52
1	A	103	SER	C-OXT	7.96	1.38	1.23
1	B	103	SER	C-OXT	7.96	1.38	1.23
1	A	21	GLU	CB-CG	7.95	1.67	1.52
1	B	21	GLU	CB-CG	7.95	1.67	1.52
1	A	71	PRO	N-CD	7.93	1.58	1.47
1	B	71	PRO	N-CD	7.93	1.58	1.47
1	A	80	MET	CG-SD	7.92	2.01	1.81
1	B	80	MET	CG-SD	7.92	2.01	1.81
1	A	16	GLN	CG-CD	7.87	1.69	1.51
1	B	16	GLN	CG-CD	7.87	1.69	1.51
1	A	59	TRP	CA-CB	-7.82	1.36	1.53
1	A	82	PHE	CA-CB	-7.82	1.36	1.53
1	B	59	TRP	CA-CB	-7.82	1.36	1.53
1	B	82	PHE	CA-CB	-7.82	1.36	1.53
1	A	72	LYS	CE-NZ	7.80	1.68	1.49
1	B	72	LYS	CE-NZ	7.80	1.68	1.49
1	A	12	GLN	C-N	-7.73	1.16	1.34
1	B	12	GLN	C-N	-7.73	1.16	1.34
1	A	11	VAL	CA-C	7.66	1.72	1.52
1	B	11	VAL	CA-C	7.66	1.72	1.52
1	A	3	VAL	C-O	-7.64	1.08	1.23
1	A	48	TYR	C-O	-7.64	1.08	1.23
1	A	63	THR	C-O	-7.64	1.08	1.23
1	B	3	VAL	C-O	-7.64	1.08	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	48	TYR	C-O	-7.64	1.08	1.23
1	B	63	THR	C-O	-7.64	1.08	1.23
1	A	9	THR	N-CA	7.61	1.61	1.46
1	B	9	THR	N-CA	7.61	1.61	1.46
1	A	27	LYS	CG-CD	-7.60	1.26	1.52
1	B	27	LYS	CG-CD	-7.60	1.26	1.52
1	A	82	PHE	CB-CG	7.59	1.64	1.51
1	B	82	PHE	CB-CG	7.59	1.64	1.51
1	A	38	ARG	CA-CB	-7.56	1.37	1.53
1	A	69	GLU	CA-CB	-7.56	1.37	1.53
1	B	38	ARG	CA-CB	-7.56	1.37	1.53
1	B	69	GLU	CA-CB	-7.56	1.37	1.53
1	A	81	ILE	CA-CB	-7.56	1.37	1.54
1	B	81	ILE	CA-CB	-7.56	1.37	1.54
1	A	79	LYS	CE-NZ	-7.55	1.30	1.49
1	B	79	LYS	CE-NZ	-7.55	1.30	1.49
1	A	34	GLY	C-O	7.54	1.35	1.23
1	A	91	ARG	C-O	-7.54	1.09	1.23
1	B	34	GLY	C-O	7.54	1.35	1.23
1	B	91	ARG	C-O	-7.54	1.09	1.23
1	A	7	LYS	CD-CE	7.53	1.70	1.51
1	B	7	LYS	CD-CE	7.53	1.70	1.51
1	A	97	TYR	CD2-CE2	7.50	1.50	1.39
1	B	97	TYR	CD2-CE2	7.50	1.50	1.39
1	A	36	PHE	CA-CB	7.49	1.70	1.53
1	B	36	PHE	CA-CB	7.49	1.70	1.53
1	A	25	LYS	CD-CE	7.49	1.70	1.51
1	B	25	LYS	CD-CE	7.49	1.70	1.51
1	A	75	ILE	C-N	7.48	1.48	1.34
1	B	75	ILE	C-N	7.48	1.48	1.34
1	A	5	LYS	CE-NZ	7.47	1.67	1.49
1	B	5	LYS	CE-NZ	7.47	1.67	1.49
1	A	19	THR	C-N	-7.43	1.17	1.34
1	B	19	THR	C-N	-7.43	1.17	1.34
1	A	18	HIS	C-O	7.43	1.37	1.23
1	B	18	HIS	C-O	7.43	1.37	1.23
1	A	98	LEU	CA-CB	-7.40	1.36	1.53
1	B	98	LEU	CA-CB	-7.40	1.36	1.53
1	A	42	GLN	CB-CG	-7.39	1.32	1.52
1	B	42	GLN	CB-CG	-7.39	1.32	1.52
1	A	47	SER	CA-CB	-7.38	1.41	1.52
1	B	47	SER	CA-CB	-7.38	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	88	LYS	C-N	7.36	1.46	1.33
1	B	88	LYS	C-N	7.36	1.46	1.33
1	A	67	TYR	CZ-OH	-7.36	1.25	1.37
1	B	67	TYR	CZ-OH	-7.36	1.25	1.37
1	A	32	LEU	CG-CD2	-7.34	1.24	1.51
1	B	32	LEU	CG-CD2	-7.34	1.24	1.51
1	A	32	LEU	CA-CB	-7.33	1.36	1.53
1	B	32	LEU	CA-CB	-7.33	1.36	1.53
1	A	76	PRO	CB-CG	-7.33	1.13	1.50
1	B	76	PRO	CB-CG	-7.33	1.13	1.50
1	A	54	SER	C-N	-7.28	1.17	1.34
1	B	54	SER	C-N	-7.28	1.17	1.34
1	A	74	TYR	CE1-CZ	-7.27	1.29	1.38
1	A	97	TYR	CE1-CZ	-7.27	1.29	1.38
1	B	74	TYR	CE1-CZ	-7.27	1.29	1.38
1	B	97	TYR	CE1-CZ	-7.27	1.29	1.38
1	A	83	ALA	C-O	-7.25	1.09	1.23
1	B	83	ALA	C-O	-7.25	1.09	1.23
1	A	59	TRP	CE3-CZ3	-7.24	1.26	1.38
1	B	59	TRP	CE3-CZ3	-7.24	1.26	1.38
1	A	90	GLU	N-CA	7.24	1.60	1.46
1	B	90	GLU	N-CA	7.24	1.60	1.46
1	A	49	THR	CB-CG2	-7.23	1.28	1.52
1	B	49	THR	CB-CG2	-7.23	1.28	1.52
1	A	16	GLN	CA-CB	-7.23	1.38	1.53
1	B	16	GLN	CA-CB	-7.23	1.38	1.53
1	A	91	ARG	CG-CD	7.21	1.70	1.51
1	B	91	ARG	CG-CD	7.21	1.70	1.51
1	A	29	GLY	C-O	7.17	1.35	1.23
1	B	29	GLY	C-O	7.17	1.35	1.23
1	A	2	ASP	CA-CB	7.17	1.69	1.53
1	B	2	ASP	CA-CB	7.17	1.69	1.53
1	A	30	PRO	CG-CD	-7.14	1.27	1.50
1	B	30	PRO	CG-CD	-7.14	1.27	1.50
1	A	44	GLU	C-O	7.12	1.36	1.23
1	B	44	GLU	C-O	7.12	1.36	1.23
1	A	23	GLY	CA-C	7.07	1.63	1.51
1	B	23	GLY	CA-C	7.07	1.63	1.51
1	A	40	THR	N-CA	7.05	1.60	1.46
1	B	40	THR	N-CA	7.05	1.60	1.46
1	A	16	GLN	C-O	7.05	1.36	1.23
1	A	42	GLN	C-O	7.05	1.36	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	93	ASP	C-O	7.05	1.36	1.23
1	B	16	GLN	C-O	7.05	1.36	1.23
1	B	42	GLN	C-O	7.05	1.36	1.23
1	B	93	ASP	C-O	7.05	1.36	1.23
1	A	80	MET	N-CA	6.99	1.60	1.46
1	B	80	MET	N-CA	6.99	1.60	1.46
1	A	26	HIS	CE1-NE2	-6.97	1.16	1.32
1	B	26	HIS	CE1-NE2	-6.97	1.16	1.32
1	A	66	GLU	CG-CD	6.90	1.62	1.51
1	B	66	GLU	CG-CD	6.90	1.62	1.51
1	A	89	GLY	CA-C	6.84	1.62	1.51
1	B	89	GLY	CA-C	6.84	1.62	1.51
1	A	95	VAL	C-O	6.82	1.36	1.23
1	B	95	VAL	C-O	6.82	1.36	1.23
1	A	33	TRP	CD2-CE3	-6.78	1.30	1.40
1	B	33	TRP	CD2-CE3	-6.78	1.30	1.40
1	A	91	ARG	CA-C	6.72	1.70	1.52
1	A	99	LYS	CA-C	6.72	1.70	1.52
1	B	91	ARG	CA-C	6.72	1.70	1.52
1	B	99	LYS	CA-C	6.72	1.70	1.52
1	A	5	LYS	CG-CD	6.68	1.75	1.52
1	B	5	LYS	CG-CD	6.68	1.75	1.52
1	A	6	GLY	N-CA	6.67	1.56	1.46
1	B	6	GLY	N-CA	6.67	1.56	1.46
1	A	103	SER	CA-CB	6.64	1.62	1.52
1	B	103	SER	CA-CB	6.64	1.62	1.52
1	A	8	LYS	C-N	-6.62	1.18	1.34
1	A	35	LEU	C-N	-6.62	1.18	1.34
1	A	78	THR	C-N	-6.62	1.18	1.34
1	A	97	TYR	C-N	-6.62	1.18	1.34
1	B	8	LYS	C-N	-6.62	1.18	1.34
1	B	35	LEU	C-N	-6.62	1.18	1.34
1	B	78	THR	C-N	-6.62	1.18	1.34
1	B	97	TYR	C-N	-6.62	1.18	1.34
1	A	79	LYS	CA-C	6.59	1.70	1.52
1	B	79	LYS	CA-C	6.59	1.70	1.52
1	A	3	VAL	N-CA	6.55	1.59	1.46
1	B	3	VAL	N-CA	6.55	1.59	1.46
1	A	60	ASN	CA-C	6.54	1.70	1.52
1	A	61	GLU	CA-C	6.54	1.70	1.52
1	B	60	ASN	CA-C	6.54	1.70	1.52
1	B	61	GLU	CA-C	6.54	1.70	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	37	GLY	C-O	6.53	1.34	1.23
1	B	37	GLY	C-O	6.53	1.34	1.23
1	A	18	HIS	CE1-NE2	6.53	1.47	1.32
1	B	18	HIS	CE1-NE2	6.53	1.47	1.32
1	A	85	ILE	CB-CG1	6.51	1.72	1.54
1	B	85	ILE	CB-CG1	6.51	1.72	1.54
1	A	78	THR	C-O	6.51	1.35	1.23
1	B	78	THR	C-O	6.51	1.35	1.23
1	A	38	ARG	C-O	-6.49	1.11	1.23
1	B	38	ARG	C-O	-6.49	1.11	1.23
1	A	74	TYR	CG-CD1	-6.43	1.30	1.39
1	B	74	TYR	CG-CD1	-6.43	1.30	1.39
1	A	61	GLU	C-N	-6.41	1.19	1.34
1	A	101	ALA	C-N	-6.41	1.19	1.34
1	A	102	THR	C-N	-6.41	1.19	1.34
1	B	61	GLU	C-N	-6.41	1.19	1.34
1	B	101	ALA	C-N	-6.41	1.19	1.34
1	B	102	THR	C-N	-6.41	1.19	1.34
1	A	59	TRP	CZ2-CH2	-6.40	1.25	1.37
1	B	59	TRP	CZ2-CH2	-6.40	1.25	1.37
1	A	74	TYR	CZ-OH	-6.34	1.27	1.37
1	A	97	TYR	CZ-OH	-6.34	1.27	1.37
1	B	74	TYR	CZ-OH	-6.34	1.27	1.37
1	B	97	TYR	CZ-OH	-6.34	1.27	1.37
1	A	27	LYS	CE-NZ	-6.28	1.33	1.49
1	B	27	LYS	CE-NZ	-6.28	1.33	1.49
1	A	11	VAL	CA-CB	-6.26	1.41	1.54
1	B	11	VAL	CA-CB	-6.26	1.41	1.54
1	A	96	ALA	N-CA	6.24	1.58	1.46
1	B	96	ALA	N-CA	6.24	1.58	1.46
1	A	62	ASN	CB-CG	-6.22	1.36	1.51
1	B	62	ASN	CB-CG	-6.22	1.36	1.51
1	A	36	PHE	CE1-CZ	6.13	1.49	1.37
1	B	36	PHE	CE1-CZ	6.13	1.49	1.37
1	A	89	GLY	C-O	-6.12	1.13	1.23
1	B	89	GLY	C-O	-6.12	1.13	1.23
1	A	53	LYS	C-O	6.12	1.34	1.23
1	B	53	LYS	C-O	6.12	1.34	1.23
1	A	26	HIS	C-N	-6.12	1.20	1.34
1	A	50	ASP	C-N	-6.12	1.20	1.34
1	A	54	SER	C-O	-6.12	1.11	1.23
1	A	97	TYR	CB-CG	6.12	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	26	HIS	C-N	-6.12	1.20	1.34
1	B	50	ASP	C-N	-6.12	1.20	1.34
1	B	54	SER	C-O	-6.12	1.11	1.23
1	B	97	TYR	CB-CG	6.12	1.60	1.51
1	A	86	LYS	CE-NZ	6.08	1.64	1.49
1	B	86	LYS	CE-NZ	6.08	1.64	1.49
1	A	20	VAL	CA-C	6.05	1.68	1.52
1	B	20	VAL	CA-C	6.05	1.68	1.52
1	A	31	ASN	C-N	-6.04	1.20	1.34
1	A	80	MET	C-N	-6.04	1.20	1.34
1	B	31	ASN	C-N	-6.04	1.20	1.34
1	B	80	MET	C-N	-6.04	1.20	1.34
1	A	76	PRO	N-CD	6.04	1.56	1.47
1	B	76	PRO	N-CD	6.04	1.56	1.47
1	A	80	MET	C-O	-6.02	1.11	1.23
1	B	80	MET	C-O	-6.02	1.11	1.23
1	A	17	CYS	CB-SG	6.01	1.92	1.82
1	B	17	CYS	CB-SG	6.01	1.92	1.82
1	A	31	ASN	CB-CG	6.00	1.64	1.51
1	B	31	ASN	CB-CG	6.00	1.64	1.51
1	A	80	MET	SD-CE	-6.00	1.44	1.77
1	B	80	MET	SD-CE	-6.00	1.44	1.77
1	A	69	GLU	N-CA	5.99	1.58	1.46
1	B	69	GLU	N-CA	5.99	1.58	1.46
1	A	10	PHE	CE1-CZ	-5.99	1.25	1.37
1	B	10	PHE	CE1-CZ	-5.99	1.25	1.37
1	A	24	GLY	C-N	5.98	1.47	1.34
1	B	24	GLY	C-N	5.98	1.47	1.34
1	A	27	LYS	CD-CE	5.97	1.66	1.51
1	B	27	LYS	CD-CE	5.97	1.66	1.51
1	A	13	LYS	CE-NZ	5.93	1.63	1.49
1	B	13	LYS	CE-NZ	5.93	1.63	1.49
1	A	55	LYS	CB-CG	5.93	1.68	1.52
1	B	55	LYS	CB-CG	5.93	1.68	1.52
1	A	69	GLU	CG-CD	5.92	1.60	1.51
1	B	69	GLU	CG-CD	5.92	1.60	1.51
1	A	12	GLN	CA-C	5.91	1.68	1.52
1	B	12	GLN	CA-C	5.91	1.68	1.52
1	A	36	PHE	CB-CG	-5.90	1.41	1.51
1	B	36	PHE	CB-CG	-5.90	1.41	1.51
1	A	92	GLN	CG-CD	5.84	1.64	1.51
1	B	92	GLN	CG-CD	5.84	1.64	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	25	LYS	CB-CG	5.84	1.68	1.52
1	B	25	LYS	CB-CG	5.84	1.68	1.52
1	A	73	LYS	CG-CD	-5.84	1.32	1.52
1	B	73	LYS	CG-CD	-5.84	1.32	1.52
1	A	81	ILE	C-N	-5.83	1.20	1.34
1	B	81	ILE	C-N	-5.83	1.20	1.34
1	A	52	ASN	CG-ND2	5.82	1.47	1.32
1	A	70	ASN	CG-ND2	5.82	1.47	1.32
1	B	52	ASN	CG-ND2	5.82	1.47	1.32
1	B	70	ASN	CG-ND2	5.82	1.47	1.32
1	A	4	ALA	N-CA	5.80	1.57	1.46
1	A	10	PHE	C-N	5.80	1.47	1.34
1	A	67	TYR	N-CA	5.80	1.57	1.46
1	B	4	ALA	N-CA	5.80	1.57	1.46
1	B	10	PHE	C-N	5.80	1.47	1.34
1	B	67	TYR	N-CA	5.80	1.57	1.46
1	A	20	VAL	CA-CB	-5.79	1.42	1.54
1	B	20	VAL	CA-CB	-5.79	1.42	1.54
1	A	27	LYS	CA-CB	5.78	1.66	1.53
1	B	27	LYS	CA-CB	5.78	1.66	1.53
1	A	33	TRP	CE3-CZ3	-5.77	1.28	1.38
1	B	33	TRP	CE3-CZ3	-5.77	1.28	1.38
1	A	65	MET	CG-SD	-5.76	1.66	1.81
1	B	65	MET	CG-SD	-5.76	1.66	1.81
1	A	11	VAL	C-N	-5.76	1.20	1.34
1	B	11	VAL	C-N	-5.76	1.20	1.34
1	A	48	TYR	CA-C	-5.73	1.38	1.52
1	B	48	TYR	CA-C	-5.73	1.38	1.52
1	A	36	PHE	CG-CD2	-5.72	1.30	1.38
1	B	36	PHE	CG-CD2	-5.72	1.30	1.38
1	A	81	ILE	CB-CG2	5.71	1.70	1.52
1	B	81	ILE	CB-CG2	5.71	1.70	1.52
1	A	90	GLU	CB-CG	-5.70	1.41	1.52
1	B	90	GLU	CB-CG	-5.70	1.41	1.52
1	A	64	LEU	CG-CD2	-5.69	1.30	1.51
1	B	64	LEU	CG-CD2	-5.69	1.30	1.51
1	A	95	VAL	CB-CG1	-5.69	1.40	1.52
1	B	95	VAL	CB-CG1	-5.69	1.40	1.52
1	A	3	VAL	C-N	-5.68	1.21	1.34
1	A	23	GLY	C-N	5.68	1.43	1.33
1	A	75	ILE	N-CA	-5.68	1.34	1.46
1	B	3	VAL	C-N	-5.68	1.21	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	23	GLY	C-N	5.68	1.43	1.33
1	B	75	ILE	N-CA	-5.68	1.34	1.46
1	A	30	PRO	C-O	-5.67	1.11	1.23
1	B	30	PRO	C-O	-5.67	1.11	1.23
1	A	25	LYS	CE-NZ	-5.63	1.34	1.49
1	B	25	LYS	CE-NZ	-5.63	1.34	1.49
1	A	38	ARG	CD-NE	-5.63	1.36	1.46
1	B	38	ARG	CD-NE	-5.63	1.36	1.46
1	A	28	VAL	CB-CG1	-5.62	1.41	1.52
1	B	28	VAL	CB-CG1	-5.62	1.41	1.52
1	A	59	TRP	CB-CG	-5.59	1.40	1.50
1	B	59	TRP	CB-CG	-5.59	1.40	1.50
1	A	90	GLU	CG-CD	5.58	1.60	1.51
1	B	90	GLU	CG-CD	5.58	1.60	1.51
1	A	95	VAL	N-CA	5.55	1.57	1.46
1	B	95	VAL	N-CA	5.55	1.57	1.46
1	A	13	LYS	CA-CB	-5.48	1.41	1.53
1	A	92	GLN	CA-CB	-5.48	1.41	1.53
1	B	13	LYS	CA-CB	-5.48	1.41	1.53
1	B	92	GLN	CA-CB	-5.48	1.41	1.53
1	A	71	PRO	CG-CD	-5.47	1.32	1.50
1	B	71	PRO	CG-CD	-5.47	1.32	1.50
1	A	12	GLN	CD-NE2	-5.41	1.19	1.32
1	B	12	GLN	CD-NE2	-5.41	1.19	1.32
1	A	39	LYS	CA-CB	5.39	1.65	1.53
1	B	39	LYS	CA-CB	5.39	1.65	1.53
1	A	65	MET	C-O	-5.37	1.13	1.23
1	B	65	MET	C-O	-5.37	1.13	1.23
1	A	53	LYS	CE-NZ	-5.33	1.35	1.49
1	B	53	LYS	CE-NZ	-5.33	1.35	1.49
1	A	11	VAL	N-CA	-5.32	1.35	1.46
1	A	52	ASN	N-CA	-5.32	1.35	1.46
1	B	11	VAL	N-CA	-5.32	1.35	1.46
1	B	52	ASN	N-CA	-5.32	1.35	1.46
1	A	26	HIS	CG-ND1	-5.30	1.27	1.38
1	B	26	HIS	CG-ND1	-5.30	1.27	1.38
1	A	46	TYR	CB-CG	-5.30	1.43	1.51
1	B	46	TYR	CB-CG	-5.30	1.43	1.51
1	A	51	ALA	CA-CB	-5.30	1.41	1.52
1	B	51	ALA	CA-CB	-5.30	1.41	1.52
1	A	45	GLY	CA-C	5.30	1.60	1.51
1	B	45	GLY	CA-C	5.30	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	59	TRP	CD1-NE1	-5.30	1.28	1.38
1	B	59	TRP	CD1-NE1	-5.30	1.28	1.38
1	A	10	PHE	CB-CG	5.28	1.60	1.51
1	A	19	THR	CA-CB	-5.28	1.39	1.53
1	B	10	PHE	CB-CG	5.28	1.60	1.51
1	B	19	THR	CA-CB	-5.28	1.39	1.53
1	A	26	HIS	C-O	5.26	1.33	1.23
1	B	26	HIS	C-O	5.26	1.33	1.23
1	A	39	LYS	C-N	-5.26	1.22	1.34
1	A	67	TYR	C-N	-5.26	1.22	1.34
1	B	39	LYS	C-N	-5.26	1.22	1.34
1	B	67	TYR	C-N	-5.26	1.22	1.34
1	A	103	SER	N-CA	5.23	1.56	1.46
1	B	103	SER	N-CA	5.23	1.56	1.46
1	A	48	TYR	CA-CB	5.18	1.65	1.53
1	B	48	TYR	CA-CB	5.18	1.65	1.53
1	A	27	LYS	CB-CG	-5.16	1.38	1.52
1	B	27	LYS	CB-CG	-5.16	1.38	1.52
1	A	62	ASN	CA-C	5.13	1.66	1.52
1	B	62	ASN	CA-C	5.13	1.66	1.52
1	A	67	TYR	CA-C	-5.13	1.39	1.52
1	A	103	SER	CA-C	-5.13	1.39	1.52
1	B	67	TYR	CA-C	-5.13	1.39	1.52
1	B	103	SER	CA-C	-5.13	1.39	1.52
1	A	13	LYS	C-N	-5.12	1.22	1.34
1	A	15	ALA	C-N	-5.12	1.22	1.34
1	A	71	PRO	C-N	-5.12	1.22	1.34
1	B	13	LYS	C-N	-5.12	1.22	1.34
1	B	15	ALA	C-N	-5.12	1.22	1.34
1	B	71	PRO	C-N	-5.12	1.22	1.34
1	A	44	GLU	N-CA	5.10	1.56	1.46
1	B	44	GLU	N-CA	5.10	1.56	1.46
1	A	87	LYS	CE-NZ	5.10	1.61	1.49
1	B	87	LYS	CE-NZ	5.10	1.61	1.49
1	A	66	GLU	N-CA	-5.10	1.36	1.46
1	B	66	GLU	N-CA	-5.10	1.36	1.46
1	A	28	VAL	CB-CG2	-5.09	1.42	1.52
1	B	28	VAL	CB-CG2	-5.09	1.42	1.52
1	A	58	VAL	CA-C	5.09	1.66	1.52
1	A	64	LEU	CA-C	5.09	1.66	1.52
1	B	58	VAL	CA-C	5.09	1.66	1.52
1	B	64	LEU	CA-C	5.09	1.66	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4	ALA	CA-CB	5.04	1.63	1.52
1	B	4	ALA	CA-CB	5.04	1.63	1.52
1	A	74	TYR	CG-CD2	-5.04	1.32	1.39
1	B	74	TYR	CG-CD2	-5.04	1.32	1.39

All (644) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	3	VAL	CA-CB-CG2	-38.56	53.07	110.90
1	B	3	VAL	CA-CB-CG2	-38.56	53.07	110.90
1	A	3	VAL	CA-CB-CG1	-33.90	60.05	110.90
1	B	3	VAL	CA-CB-CG1	-33.90	60.05	110.90
1	A	18	HIS	CG-ND1-CE1	33.74	155.43	108.20
1	B	18	HIS	CG-ND1-CE1	33.74	155.43	108.20
1	A	97	TYR	CZ-CE2-CD2	-31.30	91.63	119.80
1	B	97	TYR	CZ-CE2-CD2	-31.30	91.63	119.80
1	A	67	TYR	CB-CG-CD1	30.40	139.24	121.00
1	B	67	TYR	CB-CG-CD1	30.40	139.24	121.00
1	A	46	TYR	CZ-CE2-CD2	-27.38	95.15	119.80
1	B	46	TYR	CZ-CE2-CD2	-27.38	95.15	119.80
1	A	67	TYR	CB-CG-CD2	-26.64	105.01	121.00
1	B	67	TYR	CB-CG-CD2	-26.64	105.01	121.00
1	A	18	HIS	ND1-CG-CD2	-26.64	68.71	106.00
1	B	18	HIS	ND1-CG-CD2	-26.64	68.71	106.00
1	A	48	TYR	CB-CG-CD1	24.73	135.84	121.00
1	B	48	TYR	CB-CG-CD1	24.73	135.84	121.00
1	A	46	TYR	CB-CG-CD2	22.96	134.78	121.00
1	B	46	TYR	CB-CG-CD2	22.96	134.78	121.00
1	A	46	TYR	CG-CD2-CE2	22.32	139.16	121.30
1	B	46	TYR	CG-CD2-CE2	22.32	139.16	121.30
1	A	91	ARG	NE-CZ-NH1	-21.14	109.73	120.30
1	B	91	ARG	NE-CZ-NH1	-21.14	109.73	120.30
1	A	30	PRO	N-CD-CG	-20.85	71.93	103.20
1	B	30	PRO	N-CD-CG	-20.85	71.93	103.20
1	A	76	PRO	CA-N-CD	-20.03	83.46	111.50
1	B	76	PRO	CA-N-CD	-20.03	83.46	111.50
1	A	36	PHE	CG-CD2-CE2	19.45	142.20	120.80
1	B	36	PHE	CG-CD2-CE2	19.45	142.20	120.80
1	A	46	TYR	CB-CA-C	19.45	149.29	110.40
1	B	46	TYR	CB-CA-C	19.45	149.29	110.40
1	A	30	PRO	CA-CB-CG	-19.02	67.86	104.00
1	B	30	PRO	CA-CB-CG	-19.02	67.86	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	10	PHE	CB-CG-CD1	-19.00	107.50	120.80
1	B	10	PHE	CB-CG-CD1	-19.00	107.50	120.80
1	A	10	PHE	CZ-CE2-CD2	17.80	141.46	120.10
1	B	10	PHE	CZ-CE2-CD2	17.80	141.46	120.10
1	A	33	TRP	CG-CD2-CE3	-17.37	118.27	133.90
1	B	33	TRP	CG-CD2-CE3	-17.37	118.27	133.90
1	A	50	ASP	O-C-N	-17.14	95.28	122.70
1	B	50	ASP	O-C-N	-17.14	95.28	122.70
1	A	44	GLU	CB-CG-CD	-16.95	68.44	114.20
1	B	44	GLU	CB-CG-CD	-16.95	68.44	114.20
1	A	67	TYR	CG-CD2-CE2	-16.79	107.87	121.30
1	B	67	TYR	CG-CD2-CE2	-16.79	107.87	121.30
1	A	10	PHE	CB-CG-CD2	16.72	132.51	120.80
1	B	10	PHE	CB-CG-CD2	16.72	132.51	120.80
1	A	61	GLU	OE1-CD-OE2	-16.49	103.52	123.30
1	B	61	GLU	OE1-CD-OE2	-16.49	103.52	123.30
1	A	92	GLN	CG-CD-OE1	-16.43	88.74	121.60
1	B	92	GLN	CG-CD-OE1	-16.43	88.74	121.60
1	A	39	LYS	CA-CB-CG	16.36	149.40	113.40
1	B	39	LYS	CA-CB-CG	16.36	149.40	113.40
1	A	33	TRP	CE2-CD2-CG	15.93	120.05	107.30
1	B	33	TRP	CE2-CD2-CG	15.93	120.05	107.30
1	A	97	TYR	CG-CD2-CE2	15.86	133.99	121.30
1	B	97	TYR	CG-CD2-CE2	15.86	133.99	121.30
1	A	16	GLN	N-CA-CB	-15.47	82.75	110.60
1	B	16	GLN	N-CA-CB	-15.47	82.75	110.60
1	A	18	HIS	ND1-CE1-NE2	-15.20	76.45	109.90
1	B	18	HIS	ND1-CE1-NE2	-15.20	76.45	109.90
1	A	67	TYR	CZ-CE2-CD2	15.18	133.46	119.80
1	B	67	TYR	CZ-CE2-CD2	15.18	133.46	119.80
1	A	52	ASN	N-CA-CB	15.07	137.74	110.60
1	B	52	ASN	N-CA-CB	15.07	137.74	110.60
1	A	36	PHE	CD1-CG-CD2	-14.76	99.11	118.30
1	B	36	PHE	CD1-CG-CD2	-14.76	99.11	118.30
1	A	76	PRO	N-CD-CG	14.75	125.33	103.20
1	B	76	PRO	N-CD-CG	14.75	125.33	103.20
1	A	48	TYR	CG-CD1-CE1	14.73	133.09	121.30
1	B	48	TYR	CG-CD1-CE1	14.73	133.09	121.30
1	A	82	PHE	CB-CG-CD1	14.57	131.00	120.80
1	B	82	PHE	CB-CG-CD1	14.57	131.00	120.80
1	A	83	ALA	O-C-N	-14.21	99.03	123.20
1	B	83	ALA	O-C-N	-14.21	99.03	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	56	GLY	O-C-N	-14.14	100.08	122.70
1	B	56	GLY	O-C-N	-14.14	100.08	122.70
1	A	2	ASP	CB-CG-OD1	-14.11	105.60	118.30
1	B	2	ASP	CB-CG-OD1	-14.11	105.60	118.30
1	A	36	PHE	CB-CG-CD2	14.09	130.66	120.80
1	B	36	PHE	CB-CG-CD2	14.09	130.66	120.80
1	A	28	VAL	O-C-N	-13.62	100.05	123.20
1	B	28	VAL	O-C-N	-13.62	100.05	123.20
1	A	48	TYR	CG-CD2-CE2	13.44	132.05	121.30
1	B	48	TYR	CG-CD2-CE2	13.44	132.05	121.30
1	A	37	GLY	O-C-N	-13.43	101.20	122.70
1	B	37	GLY	O-C-N	-13.43	101.20	122.70
1	A	28	VAL	CA-CB-CG2	13.42	131.03	110.90
1	B	28	VAL	CA-CB-CG2	13.42	131.03	110.90
1	A	48	TYR	CD1-CE1-CZ	-13.30	107.83	119.80
1	B	48	TYR	CD1-CE1-CZ	-13.30	107.83	119.80
1	A	52	ASN	CB-CG-OD1	12.97	147.53	121.60
1	B	52	ASN	CB-CG-OD1	12.97	147.53	121.60
1	A	82	PHE	CD1-CG-CD2	-12.93	101.50	118.30
1	B	82	PHE	CD1-CG-CD2	-12.93	101.50	118.30
1	A	62	ASN	O-C-N	-12.89	102.07	122.70
1	B	62	ASN	O-C-N	-12.89	102.07	122.70
1	A	97	TYR	CE1-CZ-CE2	12.84	140.34	119.80
1	B	97	TYR	CE1-CZ-CE2	12.84	140.34	119.80
1	A	59	TRP	CD1-NE1-CE2	-12.75	97.52	109.00
1	B	59	TRP	CD1-NE1-CE2	-12.75	97.52	109.00
1	A	41	GLY	O-C-N	-12.70	102.37	122.70
1	B	41	GLY	O-C-N	-12.70	102.37	122.70
1	A	30	PRO	O-C-N	-12.62	102.50	122.70
1	B	30	PRO	O-C-N	-12.62	102.50	122.70
1	A	33	TRP	CB-CG-CD2	12.60	142.98	126.60
1	B	33	TRP	CB-CG-CD2	12.60	142.98	126.60
1	A	61	GLU	CG-CD-OE1	12.35	143.00	118.30
1	B	61	GLU	CG-CD-OE1	12.35	143.00	118.30
1	A	91	ARG	NE-CZ-NH2	12.35	126.47	120.30
1	B	91	ARG	NE-CZ-NH2	12.35	126.47	120.30
1	A	46	TYR	CB-CG-CD1	-12.34	113.60	121.00
1	B	46	TYR	CB-CG-CD1	-12.34	113.60	121.00
1	A	46	TYR	CA-CB-CG	12.28	136.73	113.40
1	B	46	TYR	CA-CB-CG	12.28	136.73	113.40
1	A	2	ASP	CB-CG-OD2	12.26	129.33	118.30
1	B	2	ASP	CB-CG-OD2	12.26	129.33	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	48	TYR	CD1-CG-CD2	-12.14	104.55	117.90
1	B	48	TYR	CD1-CG-CD2	-12.14	104.55	117.90
1	A	12	GLN	CG-CD-OE1	-11.99	97.62	121.60
1	B	12	GLN	CG-CD-OE1	-11.99	97.62	121.60
1	A	59	TRP	CG-CD2-CE3	-11.87	123.22	133.90
1	B	59	TRP	CG-CD2-CE3	-11.87	123.22	133.90
1	A	82	PHE	CG-CD2-CE2	11.81	133.79	120.80
1	B	82	PHE	CG-CD2-CE2	11.81	133.79	120.80
1	A	39	LYS	CA-C-N	11.65	142.82	117.20
1	B	39	LYS	CA-C-N	11.65	142.82	117.20
1	A	26	HIS	CA-CB-CG	-11.51	94.04	113.60
1	A	62	ASN	CB-CA-C	11.51	133.42	110.40
1	B	26	HIS	CA-CB-CG	-11.51	94.04	113.60
1	B	62	ASN	CB-CA-C	11.51	133.42	110.40
1	A	67	TYR	O-C-N	-11.32	104.59	122.70
1	B	67	TYR	O-C-N	-11.32	104.59	122.70
1	A	10	PHE	CE1-CZ-CE2	-11.23	99.78	120.00
1	B	10	PHE	CE1-CZ-CE2	-11.23	99.78	120.00
1	A	66	GLU	OE1-CD-OE2	-11.23	109.82	123.30
1	B	66	GLU	OE1-CD-OE2	-11.23	109.82	123.30
1	A	41	GLY	C-N-CA	11.19	149.66	121.70
1	B	41	GLY	C-N-CA	11.19	149.66	121.70
1	A	62	ASN	CA-C-O	-11.18	96.63	120.10
1	B	62	ASN	CA-C-O	-11.18	96.63	120.10
1	A	18	HIS	CG-CD2-NE2	11.08	130.25	109.20
1	B	18	HIS	CG-CD2-NE2	11.08	130.25	109.20
1	A	40	THR	O-C-N	10.99	141.88	123.20
1	B	40	THR	O-C-N	10.99	141.88	123.20
1	A	92	GLN	CB-CA-C	10.96	132.32	110.40
1	B	92	GLN	CB-CA-C	10.96	132.32	110.40
1	A	59	TRP	CD2-CE2-CZ2	-10.90	109.22	122.30
1	B	59	TRP	CD2-CE2-CZ2	-10.90	109.22	122.30
1	A	76	PRO	N-CA-CB	10.88	116.35	103.30
1	B	76	PRO	N-CA-CB	10.88	116.35	103.30
1	A	78	THR	O-C-N	-10.82	105.38	122.70
1	B	78	THR	O-C-N	-10.82	105.38	122.70
1	A	62	ASN	CA-C-N	-10.52	94.06	117.20
1	B	62	ASN	CA-C-N	-10.52	94.06	117.20
1	A	67	TYR	CA-C-O	10.51	142.17	120.10
1	B	67	TYR	CA-C-O	10.51	142.17	120.10
1	A	57	ILE	O-C-N	-10.46	105.97	122.70
1	B	57	ILE	O-C-N	-10.46	105.97	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	68	LEU	CB-CA-C	10.28	129.73	110.20
1	B	68	LEU	CB-CA-C	10.28	129.73	110.20
1	A	18	HIS	CB-CA-C	-10.20	90.00	110.40
1	B	18	HIS	CB-CA-C	-10.20	90.00	110.40
1	A	36	PHE	C-N-CA	10.15	143.62	122.30
1	B	36	PHE	C-N-CA	10.15	143.62	122.30
1	A	28	VAL	N-CA-CB	10.14	133.80	111.50
1	B	28	VAL	N-CA-CB	10.14	133.80	111.50
1	A	3	VAL	O-C-N	-10.07	106.59	122.70
1	B	3	VAL	O-C-N	-10.07	106.59	122.70
1	A	25	LYS	N-CA-CB	-10.04	92.52	110.60
1	B	25	LYS	N-CA-CB	-10.04	92.52	110.60
1	A	5	LYS	O-C-N	-10.04	106.14	123.20
1	B	5	LYS	O-C-N	-10.04	106.14	123.20
1	A	9	THR	CA-CB-CG2	10.02	126.42	112.40
1	B	9	THR	CA-CB-CG2	10.02	126.42	112.40
1	A	62	ASN	CA-CB-CG	9.87	135.12	113.40
1	B	62	ASN	CA-CB-CG	9.87	135.12	113.40
1	A	42	GLN	N-CA-CB	9.82	128.28	110.60
1	B	42	GLN	N-CA-CB	9.82	128.28	110.60
1	A	10	PHE	CG-CD1-CE1	-9.80	110.02	120.80
1	A	38	ARG	CD-NE-CZ	-9.80	109.87	123.60
1	B	10	PHE	CG-CD1-CE1	-9.80	110.02	120.80
1	B	38	ARG	CD-NE-CZ	-9.80	109.87	123.60
1	A	92	GLN	CG-CD-NE2	9.79	140.18	116.70
1	B	92	GLN	CG-CD-NE2	9.79	140.18	116.70
1	A	40	THR	C-N-CA	-9.75	101.82	122.30
1	B	40	THR	C-N-CA	-9.75	101.82	122.30
1	A	71	PRO	N-CA-CB	9.74	114.98	103.30
1	B	71	PRO	N-CA-CB	9.74	114.98	103.30
1	A	7	LYS	O-C-N	-9.65	107.25	122.70
1	B	7	LYS	O-C-N	-9.65	107.25	122.70
1	A	56	GLY	CA-C-O	9.64	137.95	120.60
1	B	56	GLY	CA-C-O	9.64	137.95	120.60
1	A	59	TRP	CE2-CD2-CE3	9.63	130.26	118.70
1	B	59	TRP	CE2-CD2-CE3	9.63	130.26	118.70
1	A	59	TRP	NE1-CE2-CZ2	-9.56	119.88	130.40
1	B	59	TRP	NE1-CE2-CZ2	-9.56	119.88	130.40
1	A	39	LYS	CA-C-O	-9.52	100.11	120.10
1	B	39	LYS	CA-C-O	-9.52	100.11	120.10
1	A	83	ALA	CA-C-O	9.48	140.02	120.10
1	B	83	ALA	CA-C-O	9.48	140.02	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	68	LEU	O-C-N	-9.47	107.55	122.70
1	B	68	LEU	O-C-N	-9.47	107.55	122.70
1	A	58	VAL	CA-C-N	9.44	137.97	117.20
1	B	58	VAL	CA-C-N	9.44	137.97	117.20
1	A	98	LEU	CB-CA-C	9.43	128.12	110.20
1	B	98	LEU	CB-CA-C	9.43	128.12	110.20
1	A	59	TRP	NE1-CE2-CD2	9.41	116.71	107.30
1	B	59	TRP	NE1-CE2-CD2	9.41	116.71	107.30
1	A	1	GLY	C-N-CA	-9.38	98.24	121.70
1	B	1	GLY	C-N-CA	-9.38	98.24	121.70
1	A	19	THR	O-C-N	-9.36	107.72	122.70
1	B	19	THR	O-C-N	-9.36	107.72	122.70
1	A	33	TRP	CD1-CG-CD2	-9.36	98.81	106.30
1	B	33	TRP	CD1-CG-CD2	-9.36	98.81	106.30
1	A	44	GLU	CG-CD-OE1	-9.30	99.70	118.30
1	B	44	GLU	CG-CD-OE1	-9.30	99.70	118.30
1	A	34	GLY	O-C-N	-9.28	107.86	122.70
1	B	34	GLY	O-C-N	-9.28	107.86	122.70
1	A	19	THR	N-CA-CB	9.22	127.82	110.30
1	B	19	THR	N-CA-CB	9.22	127.82	110.30
1	A	16	GLN	O-C-N	-9.22	107.95	122.70
1	B	16	GLN	O-C-N	-9.22	107.95	122.70
1	A	50	ASP	CA-C-N	9.21	137.46	117.20
1	B	50	ASP	CA-C-N	9.21	137.46	117.20
1	A	51	ALA	CA-C-O	9.18	139.38	120.10
1	B	51	ALA	CA-C-O	9.18	139.38	120.10
1	A	86	LYS	O-C-N	-9.11	108.12	122.70
1	B	86	LYS	O-C-N	-9.11	108.12	122.70
1	A	36	PHE	CB-CG-CD1	9.09	127.16	120.80
1	B	36	PHE	CB-CG-CD1	9.09	127.16	120.80
1	A	58	VAL	CB-CA-C	9.02	128.53	111.40
1	B	58	VAL	CB-CA-C	9.02	128.53	111.40
1	A	35	LEU	N-CA-CB	8.98	128.37	110.40
1	B	35	LEU	N-CA-CB	8.98	128.37	110.40
1	A	48	TYR	CZ-CE2-CD2	-8.89	111.80	119.80
1	B	48	TYR	CZ-CE2-CD2	-8.89	111.80	119.80
1	A	49	THR	O-C-N	-8.85	108.55	122.70
1	B	49	THR	O-C-N	-8.85	108.55	122.70
1	A	22	ASN	O-C-N	-8.80	108.24	123.20
1	B	22	ASN	O-C-N	-8.80	108.24	123.20
1	A	48	TYR	N-CA-CB	-8.78	94.79	110.60
1	B	48	TYR	N-CA-CB	-8.78	94.79	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	82	PHE	CG-CD1-CE1	8.76	130.44	120.80
1	B	82	PHE	CG-CD1-CE1	8.76	130.44	120.80
1	A	50	ASP	OD1-CG-OD2	-8.76	106.67	123.30
1	B	50	ASP	OD1-CG-OD2	-8.76	106.67	123.30
1	A	31	ASN	CA-CB-CG	-8.73	94.20	113.40
1	B	31	ASN	CA-CB-CG	-8.73	94.20	113.40
1	A	18	HIS	CA-CB-CG	-8.68	98.84	113.60
1	B	18	HIS	CA-CB-CG	-8.68	98.84	113.60
1	A	15	ALA	N-CA-C	8.66	134.37	111.00
1	B	15	ALA	N-CA-C	8.66	134.37	111.00
1	A	97	TYR	OH-CZ-CE2	-8.64	96.76	120.10
1	B	97	TYR	OH-CZ-CE2	-8.64	96.76	120.10
1	A	58	VAL	CA-C-O	-8.60	102.04	120.10
1	B	58	VAL	CA-C-O	-8.60	102.04	120.10
1	A	28	VAL	CA-C-N	8.58	133.37	116.20
1	B	28	VAL	CA-C-N	8.58	133.37	116.20
1	A	46	TYR	CD1-CG-CD2	-8.57	108.47	117.90
1	B	46	TYR	CD1-CG-CD2	-8.57	108.47	117.90
1	A	74	TYR	CD1-CE1-CZ	-8.55	112.11	119.80
1	B	74	TYR	CD1-CE1-CZ	-8.55	112.11	119.80
1	A	59	TRP	CD1-CG-CD2	-8.50	99.50	106.30
1	B	59	TRP	CD1-CG-CD2	-8.50	99.50	106.30
1	A	74	TYR	CG-CD1-CE1	8.48	128.09	121.30
1	B	74	TYR	CG-CD1-CE1	8.48	128.09	121.30
1	A	69	GLU	OE1-CD-OE2	-8.42	113.20	123.30
1	B	69	GLU	OE1-CD-OE2	-8.42	113.20	123.30
1	A	16	GLN	CA-CB-CG	8.41	131.91	113.40
1	B	16	GLN	CA-CB-CG	8.41	131.91	113.40
1	A	54	SER	O-C-N	-8.41	109.25	122.70
1	B	54	SER	O-C-N	-8.41	109.25	122.70
1	A	42	GLN	CG-CD-OE1	8.40	138.39	121.60
1	B	42	GLN	CG-CD-OE1	8.40	138.39	121.60
1	A	26	HIS	N-CA-CB	-8.34	95.58	110.60
1	B	26	HIS	N-CA-CB	-8.34	95.58	110.60
1	A	38	ARG	NE-CZ-NH1	8.31	124.46	120.30
1	B	38	ARG	NE-CZ-NH1	8.31	124.46	120.30
1	A	30	PRO	CA-C-O	8.30	140.13	120.20
1	B	30	PRO	CA-C-O	8.30	140.13	120.20
1	A	5	LYS	CB-CA-C	-8.29	93.81	110.40
1	B	5	LYS	CB-CA-C	-8.29	93.81	110.40
1	A	33	TRP	CD2-CE3-CZ3	-8.25	108.08	118.80
1	B	33	TRP	CD2-CE3-CZ3	-8.25	108.08	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	39	LYS	CB-CG-CD	8.22	132.96	111.60
1	B	39	LYS	CB-CG-CD	8.22	132.96	111.60
1	A	76	PRO	O-C-N	-8.21	109.25	123.20
1	B	76	PRO	O-C-N	-8.21	109.25	123.20
1	A	51	ALA	N-CA-CB	8.20	121.57	110.10
1	B	51	ALA	N-CA-CB	8.20	121.57	110.10
1	A	82	PHE	CB-CG-CD2	8.17	126.52	120.80
1	B	82	PHE	CB-CG-CD2	8.17	126.52	120.80
1	A	36	PHE	CG-CD1-CE1	8.17	129.78	120.80
1	B	36	PHE	CG-CD1-CE1	8.17	129.78	120.80
1	A	93	ASP	N-CA-CB	-8.12	95.97	110.60
1	B	93	ASP	N-CA-CB	-8.12	95.97	110.60
1	A	63	THR	O-C-N	-8.08	109.77	122.70
1	B	63	THR	O-C-N	-8.08	109.77	122.70
1	A	33	TRP	O-C-N	8.07	136.93	123.20
1	B	33	TRP	O-C-N	8.07	136.93	123.20
1	A	17	CYS	N-CA-C	-8.05	89.26	111.00
1	B	17	CYS	N-CA-C	-8.05	89.26	111.00
1	A	90	GLU	OE1-CD-OE2	-8.01	113.68	123.30
1	B	90	GLU	OE1-CD-OE2	-8.01	113.68	123.30
1	A	36	PHE	N-CA-CB	-8.00	96.19	110.60
1	B	36	PHE	N-CA-CB	-8.00	96.19	110.60
1	A	6	GLY	N-CA-C	-7.99	93.12	113.10
1	B	6	GLY	N-CA-C	-7.99	93.12	113.10
1	A	31	ASN	O-C-N	-7.96	109.97	122.70
1	B	31	ASN	O-C-N	-7.96	109.97	122.70
1	A	32	LEU	N-CA-CB	7.94	126.29	110.40
1	B	32	LEU	N-CA-CB	7.94	126.29	110.40
1	A	75	ILE	C-N-CD	7.90	144.98	128.40
1	B	75	ILE	C-N-CD	7.90	144.98	128.40
1	A	33	TRP	N-CA-CB	7.87	124.76	110.60
1	B	33	TRP	N-CA-CB	7.87	124.76	110.60
1	A	88	LYS	O-C-N	-7.86	109.83	123.20
1	B	88	LYS	O-C-N	-7.86	109.83	123.20
1	A	40	THR	CA-CB-CG2	-7.85	101.41	112.40
1	B	40	THR	CA-CB-CG2	-7.85	101.41	112.40
1	A	86	LYS	CA-C-O	7.84	136.57	120.10
1	B	86	LYS	CA-C-O	7.84	136.57	120.10
1	A	62	ASN	OD1-CG-ND2	-7.81	103.93	121.90
1	B	62	ASN	OD1-CG-ND2	-7.81	103.93	121.90
1	A	43	ALA	O-C-N	-7.79	110.24	122.70
1	B	43	ALA	O-C-N	-7.79	110.24	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	97	TYR	O-C-N	-7.74	110.32	122.70
1	B	97	TYR	O-C-N	-7.74	110.32	122.70
1	A	44	GLU	O-C-N	-7.74	110.05	123.20
1	B	44	GLU	O-C-N	-7.74	110.05	123.20
1	A	97	TYR	N-CA-CB	7.70	124.46	110.60
1	B	97	TYR	N-CA-CB	7.70	124.46	110.60
1	A	79	LYS	O-C-N	-7.69	110.40	122.70
1	B	79	LYS	O-C-N	-7.69	110.40	122.70
1	A	33	TRP	CH2-CZ2-CE2	7.65	125.05	117.40
1	B	33	TRP	CH2-CZ2-CE2	7.65	125.05	117.40
1	A	77	GLY	CA-C-O	7.63	134.34	120.60
1	B	77	GLY	CA-C-O	7.63	134.34	120.60
1	A	10	PHE	CA-C-N	7.58	133.88	117.20
1	B	10	PHE	CA-C-N	7.58	133.88	117.20
1	A	99	LYS	CD-CE-NZ	7.54	129.04	111.70
1	B	99	LYS	CD-CE-NZ	7.54	129.04	111.70
1	A	33	TRP	CA-CB-CG	7.53	128.00	113.70
1	B	33	TRP	CA-CB-CG	7.53	128.00	113.70
1	A	74	TYR	CZ-CE2-CD2	-7.49	113.06	119.80
1	B	74	TYR	CZ-CE2-CD2	-7.49	113.06	119.80
1	A	38	ARG	CA-C-N	-7.45	100.81	117.20
1	B	38	ARG	CA-C-N	-7.45	100.81	117.20
1	A	79	LYS	CD-CE-NZ	7.45	128.82	111.70
1	B	79	LYS	CD-CE-NZ	7.45	128.82	111.70
1	A	45	GLY	CA-C-N	7.44	133.56	117.20
1	B	45	GLY	CA-C-N	7.44	133.56	117.20
1	A	74	TYR	CG-CD2-CE2	7.38	127.20	121.30
1	B	74	TYR	CG-CD2-CE2	7.38	127.20	121.30
1	A	58	VAL	N-CA-C	-7.35	91.15	111.00
1	B	58	VAL	N-CA-C	-7.35	91.15	111.00
1	A	78	THR	CA-C-N	7.33	133.32	117.20
1	B	78	THR	CA-C-N	7.33	133.32	117.20
1	A	66	GLU	N-CA-CB	7.33	123.79	110.60
1	B	66	GLU	N-CA-CB	7.33	123.79	110.60
1	A	13	LYS	N-CA-CB	-7.33	97.42	110.60
1	B	13	LYS	N-CA-CB	-7.33	97.42	110.60
1	A	38	ARG	CB-CA-C	-7.31	95.78	110.40
1	B	38	ARG	CB-CA-C	-7.31	95.78	110.40
1	A	46	TYR	CE1-CZ-CE2	7.29	131.47	119.80
1	B	46	TYR	CE1-CZ-CE2	7.29	131.47	119.80
1	A	90	GLU	O-C-N	-7.28	111.05	122.70
1	B	90	GLU	O-C-N	-7.28	111.05	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	5	LYS	CA-CB-CG	7.25	129.35	113.40
1	B	5	LYS	CA-CB-CG	7.25	129.35	113.40
1	A	40	THR	CA-C-O	-7.24	104.89	120.10
1	B	40	THR	CA-C-O	-7.24	104.89	120.10
1	A	31	ASN	OD1-CG-ND2	-7.24	105.25	121.90
1	A	40	THR	OG1-CB-CG2	-7.24	93.35	110.00
1	B	31	ASN	OD1-CG-ND2	-7.24	105.25	121.90
1	B	40	THR	OG1-CB-CG2	-7.24	93.35	110.00
1	A	63	THR	CA-C-O	7.22	135.26	120.10
1	B	63	THR	CA-C-O	7.22	135.26	120.10
1	A	44	GLU	CB-CA-C	7.07	124.54	110.40
1	B	44	GLU	CB-CA-C	7.07	124.54	110.40
1	A	29	GLY	CA-C-O	-7.02	107.97	120.60
1	B	29	GLY	CA-C-O	-7.02	107.97	120.60
1	A	62	ASN	CB-CG-ND2	6.96	133.42	116.70
1	B	62	ASN	CB-CG-ND2	6.96	133.42	116.70
1	A	18	HIS	CB-CG-ND1	6.95	140.57	123.20
1	B	18	HIS	CB-CG-ND1	6.95	140.57	123.20
1	A	12	GLN	CB-CG-CD	6.95	129.66	111.60
1	B	12	GLN	CB-CG-CD	6.95	129.66	111.60
1	A	97	TYR	CG-CD1-CE1	-6.94	115.75	121.30
1	B	97	TYR	CG-CD1-CE1	-6.94	115.75	121.30
1	A	58	VAL	O-C-N	-6.94	111.59	122.70
1	B	58	VAL	O-C-N	-6.94	111.59	122.70
1	A	55	LYS	O-C-N	6.89	134.91	123.20
1	B	55	LYS	O-C-N	6.89	134.91	123.20
1	A	48	TYR	CB-CA-C	6.88	124.16	110.40
1	B	48	TYR	CB-CA-C	6.88	124.16	110.40
1	A	6	GLY	O-C-N	-6.87	111.72	122.70
1	B	6	GLY	O-C-N	-6.87	111.72	122.70
1	A	84	GLY	N-CA-C	6.86	130.24	113.10
1	B	84	GLY	N-CA-C	6.86	130.24	113.10
1	A	77	GLY	O-C-N	-6.84	111.75	122.70
1	B	77	GLY	O-C-N	-6.84	111.75	122.70
1	A	66	GLU	CG-CD-OE2	6.83	131.96	118.30
1	B	66	GLU	CG-CD-OE2	6.83	131.96	118.30
1	A	33	TRP	CB-CG-CD1	-6.76	118.20	127.00
1	A	83	ALA	CB-CA-C	-6.76	99.95	110.10
1	B	33	TRP	CB-CG-CD1	-6.76	118.20	127.00
1	B	83	ALA	CB-CA-C	-6.76	99.95	110.10
1	A	69	GLU	C-N-CA	-6.75	104.81	121.70
1	B	69	GLU	C-N-CA	-6.75	104.81	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	93	ASP	OD1-CG-OD2	-6.73	110.51	123.30
1	B	93	ASP	OD1-CG-OD2	-6.73	110.51	123.30
1	A	74	TYR	CD1-CG-CD2	-6.72	110.50	117.90
1	B	74	TYR	CD1-CG-CD2	-6.72	110.50	117.90
1	A	58	VAL	N-CA-CB	6.72	126.28	111.50
1	B	58	VAL	N-CA-CB	6.72	126.28	111.50
1	A	38	ARG	N-CA-C	-6.71	92.89	111.00
1	B	38	ARG	N-CA-C	-6.71	92.89	111.00
1	A	15	ALA	N-CA-CB	-6.70	100.72	110.10
1	B	15	ALA	N-CA-CB	-6.70	100.72	110.10
1	A	93	ASP	CA-CB-CG	6.66	128.06	113.40
1	B	93	ASP	CA-CB-CG	6.66	128.06	113.40
1	A	16	GLN	C-N-CA	-6.66	105.05	121.70
1	B	16	GLN	C-N-CA	-6.66	105.05	121.70
1	A	81	ILE	CB-CA-C	6.66	124.92	111.60
1	B	81	ILE	CB-CA-C	6.66	124.92	111.60
1	A	45	GLY	CA-C-O	-6.64	108.64	120.60
1	B	45	GLY	CA-C-O	-6.64	108.64	120.60
1	A	93	ASP	O-C-N	-6.63	112.09	122.70
1	B	93	ASP	O-C-N	-6.63	112.09	122.70
1	A	12	GLN	CA-C-N	6.60	131.72	117.20
1	B	12	GLN	CA-C-N	6.60	131.72	117.20
1	A	16	GLN	CB-CG-CD	-6.58	94.49	111.60
1	B	16	GLN	CB-CG-CD	-6.58	94.49	111.60
1	A	79	LYS	CA-C-O	6.55	133.86	120.10
1	B	79	LYS	CA-C-O	6.55	133.86	120.10
1	A	37	GLY	CA-C-O	6.52	132.33	120.60
1	B	37	GLY	CA-C-O	6.52	132.33	120.60
1	A	38	ARG	CA-C-O	6.48	133.71	120.10
1	B	38	ARG	CA-C-O	6.48	133.71	120.10
1	A	2	ASP	CA-CB-CG	6.48	127.65	113.40
1	B	2	ASP	CA-CB-CG	6.48	127.65	113.40
1	A	46	TYR	N-CA-C	-6.45	93.57	111.00
1	B	46	TYR	N-CA-C	-6.45	93.57	111.00
1	A	79	LYS	N-CA-CB	6.41	122.14	110.60
1	B	79	LYS	N-CA-CB	6.41	122.14	110.60
1	A	51	ALA	CB-CA-C	-6.36	100.56	110.10
1	B	51	ALA	CB-CA-C	-6.36	100.56	110.10
1	A	55	LYS	CB-CG-CD	-6.32	95.16	111.60
1	B	55	LYS	CB-CG-CD	-6.32	95.16	111.60
1	A	35	LEU	CA-C-O	6.32	133.37	120.10
1	B	35	LEU	CA-C-O	6.32	133.37	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	19	THR	OG1-CB-CG2	6.31	124.52	110.00
1	B	19	THR	OG1-CB-CG2	6.31	124.52	110.00
1	A	33	TRP	NE1-CE2-CZ2	6.31	137.34	130.40
1	B	33	TRP	NE1-CE2-CZ2	6.31	137.34	130.40
1	A	36	PHE	CD1-CE1-CZ	-6.31	112.53	120.10
1	B	36	PHE	CD1-CE1-CZ	-6.31	112.53	120.10
1	A	36	PHE	O-C-N	-6.30	112.49	123.20
1	B	36	PHE	O-C-N	-6.30	112.49	123.20
1	A	10	PHE	CA-C-O	-6.29	106.89	120.10
1	B	10	PHE	CA-C-O	-6.29	106.89	120.10
1	A	93	ASP	CB-CG-OD2	6.28	123.95	118.30
1	B	93	ASP	CB-CG-OD2	6.28	123.95	118.30
1	A	57	ILE	CA-C-O	6.21	133.14	120.10
1	B	57	ILE	CA-C-O	6.21	133.14	120.10
1	A	54	SER	CA-C-N	6.20	130.83	117.20
1	B	54	SER	CA-C-N	6.20	130.83	117.20
1	A	60	ASN	N-CA-CB	6.19	121.75	110.60
1	B	60	ASN	N-CA-CB	6.19	121.75	110.60
1	A	34	GLY	CA-C-O	6.19	131.74	120.60
1	B	34	GLY	CA-C-O	6.19	131.74	120.60
1	A	59	TRP	O-C-N	6.18	132.59	122.70
1	B	59	TRP	O-C-N	6.18	132.59	122.70
1	A	94	LEU	CB-CG-CD2	6.11	121.39	111.00
1	B	94	LEU	CB-CG-CD2	6.11	121.39	111.00
1	A	42	GLN	CB-CG-CD	6.06	127.35	111.60
1	A	74	TYR	CB-CG-CD2	6.06	124.63	121.00
1	B	42	GLN	CB-CG-CD	6.06	127.35	111.60
1	B	74	TYR	CB-CG-CD2	6.06	124.63	121.00
1	A	71	PRO	C-N-CA	6.01	136.72	121.70
1	B	71	PRO	C-N-CA	6.01	136.72	121.70
1	A	47	SER	N-CA-CB	6.00	119.51	110.50
1	A	74	TYR	CB-CG-CD1	6.00	124.60	121.00
1	B	47	SER	N-CA-CB	6.00	119.51	110.50
1	B	74	TYR	CB-CG-CD1	6.00	124.60	121.00
1	A	63	THR	CA-CB-CG2	-5.99	104.01	112.40
1	B	63	THR	CA-CB-CG2	-5.99	104.01	112.40
1	A	79	LYS	CA-CB-CG	-5.93	100.36	113.40
1	B	79	LYS	CA-CB-CG	-5.93	100.36	113.40
1	A	67	TYR	N-CA-CB	-5.92	99.95	110.60
1	B	67	TYR	N-CA-CB	-5.92	99.95	110.60
1	A	91	ARG	N-CA-C	-5.91	95.05	111.00
1	B	91	ARG	N-CA-C	-5.91	95.05	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	55	LYS	N-CA-CB	5.90	121.22	110.60
1	B	55	LYS	N-CA-CB	5.90	121.22	110.60
1	A	51	ALA	O-C-N	-5.88	113.28	122.70
1	A	69	GLU	CG-CD-OE1	5.88	130.07	118.30
1	B	51	ALA	O-C-N	-5.88	113.28	122.70
1	B	69	GLU	CG-CD-OE1	5.88	130.07	118.30
1	A	38	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	A	52	ASN	O-C-N	-5.88	113.30	122.70
1	B	38	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	B	52	ASN	O-C-N	-5.88	113.30	122.70
1	A	44	GLU	CG-CD-OE2	5.86	130.01	118.30
1	B	44	GLU	CG-CD-OE2	5.86	130.01	118.30
1	A	43	ALA	N-CA-CB	5.85	118.29	110.10
1	B	43	ALA	N-CA-CB	5.85	118.29	110.10
1	A	73	LYS	CB-CA-C	-5.83	98.74	110.40
1	A	92	GLN	O-C-N	-5.83	113.37	122.70
1	B	73	LYS	CB-CA-C	-5.83	98.74	110.40
1	B	92	GLN	O-C-N	-5.83	113.37	122.70
1	A	5	LYS	CA-C-N	5.83	127.85	116.20
1	B	5	LYS	CA-C-N	5.83	127.85	116.20
1	A	71	PRO	O-C-N	-5.82	113.38	122.70
1	B	71	PRO	O-C-N	-5.82	113.38	122.70
1	A	69	GLU	CB-CA-C	5.82	122.04	110.40
1	B	69	GLU	CB-CA-C	5.82	122.04	110.40
1	A	33	TRP	C-N-CA	-5.81	110.09	122.30
1	B	33	TRP	C-N-CA	-5.81	110.09	122.30
1	A	73	LYS	CB-CG-CD	5.80	126.68	111.60
1	B	73	LYS	CB-CG-CD	5.80	126.68	111.60
1	A	86	LYS	N-CA-C	-5.79	95.35	111.00
1	B	86	LYS	N-CA-C	-5.79	95.35	111.00
1	A	32	LEU	O-C-N	-5.79	113.43	122.70
1	B	32	LEU	O-C-N	-5.79	113.43	122.70
1	A	63	THR	CA-CB-OG1	-5.79	96.85	109.00
1	B	63	THR	CA-CB-OG1	-5.79	96.85	109.00
1	A	15	ALA	CB-CA-C	-5.75	101.47	110.10
1	B	15	ALA	CB-CA-C	-5.75	101.47	110.10
1	A	48	TYR	CA-CB-CG	5.73	124.29	113.40
1	B	48	TYR	CA-CB-CG	5.73	124.29	113.40
1	A	52	ASN	CB-CG-ND2	-5.73	102.95	116.70
1	B	52	ASN	CB-CG-ND2	-5.73	102.95	116.70
1	A	10	PHE	O-C-N	-5.70	113.59	122.70
1	B	10	PHE	O-C-N	-5.70	113.59	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	41	GLY	CA-C-N	5.69	129.72	117.20
1	A	57	ILE	CA-CB-CG2	5.69	122.29	110.90
1	B	41	GLY	CA-C-N	5.69	129.72	117.20
1	B	57	ILE	CA-CB-CG2	5.69	122.29	110.90
1	A	52	ASN	OD1-CG-ND2	-5.65	108.90	121.90
1	B	52	ASN	OD1-CG-ND2	-5.65	108.90	121.90
1	A	18	HIS	CB-CG-CD2	5.64	148.29	130.80
1	B	18	HIS	CB-CG-CD2	5.64	148.29	130.80
1	A	5	LYS	CD-CE-NZ	5.64	124.66	111.70
1	A	55	LYS	CD-CE-NZ	5.64	124.66	111.70
1	B	5	LYS	CD-CE-NZ	5.64	124.66	111.70
1	B	55	LYS	CD-CE-NZ	5.64	124.66	111.70
1	A	74	TYR	CE1-CZ-CE2	5.63	128.82	119.80
1	B	74	TYR	CE1-CZ-CE2	5.63	128.82	119.80
1	A	80	MET	CA-C-O	5.63	131.93	120.10
1	B	80	MET	CA-C-O	5.63	131.93	120.10
1	A	92	GLN	CA-C-O	5.63	131.92	120.10
1	B	92	GLN	CA-C-O	5.63	131.92	120.10
1	A	101	ALA	O-C-N	-5.61	113.72	122.70
1	B	101	ALA	O-C-N	-5.61	113.72	122.70
1	A	66	GLU	O-C-N	5.61	131.67	122.70
1	B	66	GLU	O-C-N	5.61	131.67	122.70
1	A	79	LYS	CB-CG-CD	5.59	126.14	111.60
1	B	79	LYS	CB-CG-CD	5.59	126.14	111.60
1	A	70	ASN	CA-C-O	5.58	131.81	120.10
1	B	70	ASN	CA-C-O	5.58	131.81	120.10
1	A	99	LYS	CA-C-N	5.57	129.46	117.20
1	B	99	LYS	CA-C-N	5.57	129.46	117.20
1	A	11	VAL	CG1-CB-CG2	-5.57	101.99	110.90
1	B	11	VAL	CG1-CB-CG2	-5.57	101.99	110.90
1	A	45	GLY	N-CA-C	5.55	126.97	113.10
1	B	45	GLY	N-CA-C	5.55	126.97	113.10
1	A	55	LYS	CA-C-N	-5.53	105.13	116.20
1	B	55	LYS	CA-C-N	-5.53	105.13	116.20
1	A	50	ASP	CB-CG-OD2	5.51	123.26	118.30
1	B	50	ASP	CB-CG-OD2	5.51	123.26	118.30
1	A	82	PHE	N-CA-CB	-5.50	100.69	110.60
1	B	82	PHE	N-CA-CB	-5.50	100.69	110.60
1	A	61	GLU	N-CA-C	-5.48	96.20	111.00
1	B	61	GLU	N-CA-C	-5.48	96.20	111.00
1	A	59	TRP	CA-C-O	-5.45	108.66	120.10
1	B	59	TRP	CA-C-O	-5.45	108.66	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	87	LYS	CA-CB-CG	5.43	125.36	113.40
1	B	87	LYS	CA-CB-CG	5.43	125.36	113.40
1	A	84	GLY	O-C-N	-5.42	114.03	122.70
1	B	84	GLY	O-C-N	-5.42	114.03	122.70
1	A	102	THR	CA-CB-CG2	5.41	119.97	112.40
1	B	102	THR	CA-CB-CG2	5.41	119.97	112.40
1	A	95	VAL	CA-C-N	5.41	129.09	117.20
1	B	95	VAL	CA-C-N	5.41	129.09	117.20
1	A	103	SER	CB-CA-C	5.40	120.37	110.10
1	B	103	SER	CB-CA-C	5.40	120.37	110.10
1	A	68	LEU	CD1-CG-CD2	-5.39	94.34	110.50
1	B	68	LEU	CD1-CG-CD2	-5.39	94.34	110.50
1	A	59	TRP	CE3-CZ3-CH2	5.34	127.07	121.20
1	B	59	TRP	CE3-CZ3-CH2	5.34	127.07	121.20
1	A	32	LEU	N-CA-C	-5.33	96.61	111.00
1	B	32	LEU	N-CA-C	-5.33	96.61	111.00
1	A	89	GLY	C-N-CA	5.32	135.00	121.70
1	B	89	GLY	C-N-CA	5.32	135.00	121.70
1	A	47	SER	CA-CB-OG	-5.30	96.88	111.20
1	A	52	ASN	CB-CA-C	-5.30	99.80	110.40
1	B	47	SER	CA-CB-OG	-5.30	96.88	111.20
1	B	52	ASN	CB-CA-C	-5.30	99.80	110.40
1	A	42	GLN	OE1-CD-NE2	-5.25	109.83	121.90
1	B	42	GLN	OE1-CD-NE2	-5.25	109.83	121.90
1	A	36	PHE	CZ-CE2-CD2	-5.22	113.84	120.10
1	B	36	PHE	CZ-CE2-CD2	-5.22	113.84	120.10
1	A	59	TRP	CB-CG-CD1	5.21	133.78	127.00
1	B	59	TRP	CB-CG-CD1	5.21	133.78	127.00
1	A	93	ASP	CA-C-N	5.20	128.63	117.20
1	B	93	ASP	CA-C-N	5.20	128.63	117.20
1	A	23	GLY	N-CA-C	-5.19	100.11	113.10
1	B	23	GLY	N-CA-C	-5.19	100.11	113.10
1	A	73	LYS	CG-CD-CE	5.19	127.46	111.90
1	A	101	ALA	CA-C-N	5.19	128.61	117.20
1	B	73	LYS	CG-CD-CE	5.19	127.46	111.90
1	B	101	ALA	CA-C-N	5.19	128.61	117.20
1	A	70	ASN	OD1-CG-ND2	-5.18	109.99	121.90
1	B	70	ASN	OD1-CG-ND2	-5.18	109.99	121.90
1	A	97	TYR	CA-C-O	5.11	130.84	120.10
1	B	97	TYR	CA-C-O	5.11	130.84	120.10
1	A	82	PHE	O-C-N	-5.11	114.53	122.70
1	B	82	PHE	O-C-N	-5.11	114.53	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	69	GLU	N-CA-CB	-5.09	101.44	110.60
1	B	69	GLU	N-CA-CB	-5.09	101.44	110.60
1	A	69	GLU	CA-CB-CG	5.08	124.57	113.40
1	B	69	GLU	CA-CB-CG	5.08	124.57	113.40
1	A	25	LYS	CD-CE-NZ	5.07	123.36	111.70
1	B	25	LYS	CD-CE-NZ	5.07	123.36	111.70
1	A	92	GLN	C-N-CA	-5.06	109.04	121.70
1	B	92	GLN	C-N-CA	-5.06	109.04	121.70
1	A	74	TYR	CB-CA-C	-5.06	100.28	110.40
1	B	74	TYR	CB-CA-C	-5.06	100.28	110.40
1	A	10	PHE	CB-CA-C	-5.06	100.28	110.40
1	A	22	ASN	CA-C-N	5.06	126.31	116.20
1	B	10	PHE	CB-CA-C	-5.06	100.28	110.40
1	B	22	ASN	CA-C-N	5.06	126.31	116.20
1	A	86	LYS	CB-CG-CD	5.05	124.74	111.60
1	B	86	LYS	CB-CG-CD	5.05	124.74	111.60
1	A	36	PHE	CB-CA-C	5.04	120.48	110.40
1	B	36	PHE	CB-CA-C	5.04	120.48	110.40
1	A	21	GLU	CA-CB-CG	5.02	124.45	113.40
1	B	21	GLU	CA-CB-CG	5.02	124.45	113.40
1	A	65	MET	C-N-CA	5.00	134.21	121.70
1	B	65	MET	C-N-CA	5.00	134.21	121.70

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	40	THR	CB
1	A	78	THR	CB
1	B	40	THR	CB
1	B	78	THR	CB

All (70) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	10	PHE	Mainchain
1	A	12	GLN	Sidechain
1	A	16	GLN	Sidechain
1	A	17	CYS	Mainchain
1	A	18	HIS	Sidechain
1	A	2	ASP	Mainchain
1	A	21	GLU	Mainchain
1	A	26	HIS	Sidechain

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Mol	Chain	Res	Type	Group
1	A	29	GLY	Mainchain
1	A	32	LEU	Mainchain
1	A	43	ALA	Mainchain
1	A	44	GLU	Sidechain,Mainchain
1	A	45	GLY	Mainchain
1	A	46	TYR	Sidechain
1	A	47	SER	Mainchain
1	A	49	THR	Mainchain
1	A	5	LYS	Mainchain
1	A	50	ASP	Sidechain
1	A	58	VAL	Mainchain
1	A	61	GLU	Mainchain
1	A	62	ASN	Sidechain,Mainchain
1	A	67	TYR	Sidechain
1	A	69	GLU	Mainchain
1	A	72	LYS	Mainchain
1	A	74	TYR	Mainchain
1	A	77	GLY	Mainchain
1	A	82	PHE	Mainchain
1	A	87	LYS	Mainchain
1	A	91	ARG	Sidechain
1	A	92	GLN	Sidechain
1	A	93	ASP	Sidechain
1	A	94	LEU	Mainchain
1	A	97	TYR	Sidechain
1	B	10	PHE	Mainchain
1	B	12	GLN	Sidechain
1	B	16	GLN	Sidechain
1	B	17	CYS	Mainchain
1	B	18	HIS	Sidechain
1	B	2	ASP	Mainchain
1	B	21	GLU	Mainchain
1	B	26	HIS	Sidechain
1	B	29	GLY	Mainchain
1	B	32	LEU	Mainchain
1	B	43	ALA	Mainchain
1	B	44	GLU	Sidechain,Mainchain
1	B	45	GLY	Mainchain
1	B	46	TYR	Sidechain
1	B	47	SER	Mainchain
1	B	49	THR	Mainchain
1	B	5	LYS	Mainchain

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Mol	Chain	Res	Type	Group
1	B	50	ASP	Sidechain
1	B	58	VAL	Mainchain
1	B	61	GLU	Mainchain
1	B	62	ASN	Sidechain,Mainchain
1	B	67	TYR	Sidechain
1	B	69	GLU	Mainchain
1	B	72	LYS	Mainchain
1	B	74	TYR	Mainchain
1	B	77	GLY	Mainchain
1	B	82	PHE	Mainchain
1	B	87	LYS	Mainchain
1	B	91	ARG	Sidechain
1	B	92	GLN	Sidechain
1	B	93	ASP	Sidechain
1	B	94	LEU	Mainchain
1	B	97	TYR	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	795	0	773	388	47
1	B	795	0	773	388	47
2	A	43	0	27	23	0
2	B	43	0	27	23	0
3	A	1	0	0	0	0
All	All	1677	0	1600	761	54

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 233.

All (761) 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:66:GLU:HB3	1:A:74:TYR:CE2	1.24	1.67
1:B:66:GLU:HB3	1:B:74:TYR:CE2	1.24	1.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:HIS:CB	1:A:26:HIS:CG	1.78	1.64
1:B:26:HIS:CG	1:B:26:HIS:CB	1.78	1.64
1:A:49:THR:CA	1:A:49:THR:CB	1.74	1.63
1:B:49:THR:CB	1:B:49:THR:CA	1.74	1.63
1:A:5:LYS:CD	1:A:5:LYS:CG	1.75	1.63
1:B:5:LYS:CD	1:B:5:LYS:CG	1.75	1.63
1:A:53:LYS:CD	1:A:53:LYS:CE	1.78	1.62
1:A:86:LYS:CE	1:A:86:LYS:CD	1.77	1.62
1:B:53:LYS:CE	1:B:53:LYS:CD	1.78	1.62
1:B:86:LYS:CD	1:B:86:LYS:CE	1.77	1.62
1:A:17:CYS:CB	1:A:17:CYS:CA	1.75	1.60
1:B:17:CYS:CB	1:B:17:CYS:CA	1.75	1.60
1:A:56:GLY:N	1:A:56:GLY:CA	1.68	1.56
1:B:56:GLY:CA	1:B:56:GLY:N	1.68	1.56
1:A:91:ARG:N	1:A:91:ARG:CA	1.70	1.55
1:B:91:ARG:N	1:B:91:ARG:CA	1.70	1.55
1:A:32:LEU:N	1:A:32:LEU:CA	1.68	1.55
1:B:32:LEU:N	1:B:32:LEU:CA	1.68	1.55
1:A:86:LYS:CD	1:A:86:LYS:CG	1.80	1.54
1:A:98:LEU:C	1:A:98:LEU:CA	1.75	1.54
1:B:86:LYS:CD	1:B:86:LYS:CG	1.80	1.54
1:B:98:LEU:C	1:B:98:LEU:CA	1.75	1.54
1:A:5:LYS:CE	1:A:5:LYS:NZ	1.67	1.52
1:A:62:ASN:N	1:A:62:ASN:CA	1.70	1.52
1:B:5:LYS:CE	1:B:5:LYS:NZ	1.67	1.52
1:B:62:ASN:N	1:B:62:ASN:CA	1.70	1.52
1:A:72:LYS:NZ	1:A:72:LYS:CE	1.68	1.52
1:B:72:LYS:CE	1:B:72:LYS:NZ	1.68	1.52
1:A:43:ALA:N	1:A:43:ALA:CA	1.70	1.52
1:A:59:TRP:N	1:A:59:TRP:CA	1.69	1.52
1:B:43:ALA:N	1:B:43:ALA:CA	1.70	1.52
1:B:59:TRP:CA	1:B:59:TRP:N	1.69	1.52
1:A:82:PHE:CA	1:A:82:PHE:N	1.70	1.51
1:B:82:PHE:N	1:B:82:PHE:CA	1.70	1.51
1:A:98:LEU:CA	1:A:98:LEU:N	1.73	1.51
1:B:98:LEU:CA	1:B:98:LEU:N	1.73	1.51
1:A:33:TRP:N	1:A:33:TRP:CA	1.70	1.51
1:B:33:TRP:N	1:B:33:TRP:CA	1.70	1.51
1:A:18:HIS:N	1:A:18:HIS:CA	1.68	1.50
1:A:101:ALA:N	1:A:101:ALA:CA	1.72	1.50
1:B:18:HIS:N	1:B:18:HIS:CA	1.68	1.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:ALA:CA	1:B:101:ALA:N	1.72	1.50
1:A:16:GLN:CA	1:A:16:GLN:N	1.71	1.49
1:B:16:GLN:N	1:B:16:GLN:CA	1.71	1.49
1:A:3:VAL:CA	1:A:3:VAL:C	1.79	1.48
1:B:3:VAL:C	1:B:3:VAL:CA	1.79	1.48
1:A:83:ALA:CB	1:A:83:ALA:CA	1.91	1.48
1:B:83:ALA:CA	1:B:83:ALA:CB	1.91	1.48
1:A:80:MET:CG	1:A:80:MET:SD	2.01	1.47
1:B:80:MET:CG	1:B:80:MET:SD	2.01	1.47
1:A:46:TYR:CD1	1:A:46:TYR:CB	1.97	1.46
1:B:46:TYR:CD1	1:B:46:TYR:CB	1.97	1.46
1:A:64:LEU:CB	1:A:64:LEU:CA	1.91	1.45
1:B:64:LEU:CB	1:B:64:LEU:CA	1.91	1.45
1:A:92:GLN:N	1:A:92:GLN:CA	1.76	1.45
1:B:92:GLN:CA	1:B:92:GLN:N	1.76	1.45
2:A:104:HEC:O1D	2:A:104:HEC:CGD	1.66	1.44
2:B:104:HEC:CGD	2:B:104:HEC:O1D	1.66	1.44
1:A:47:SER:CB	1:A:47:SER:OG	1.69	1.40
1:B:47:SER:CB	1:B:47:SER:OG	1.69	1.40
1:A:24:GLY:N	1:A:24:GLY:CA	1.84	1.40
1:B:24:GLY:N	1:B:24:GLY:CA	1.84	1.40
1:A:46:TYR:CD1	1:A:46:TYR:CD2	1.93	1.38
1:B:46:TYR:CD1	1:B:46:TYR:CD2	1.93	1.38
1:A:86:LYS:CE	1:B:103:SER:CA	2.01	1.38
1:A:66:GLU:HB3	1:A:74:TYR:CZ	1.57	1.38
1:B:66:GLU:HB3	1:B:74:TYR:CZ	1.57	1.38
1:A:12:GLN:CG	1:A:12:GLN:CD	1.93	1.36
1:B:12:GLN:CD	1:B:12:GLN:CG	1.93	1.36
1:A:73:LYS:CE	1:A:73:LYS:CD	2.04	1.35
1:B:73:LYS:CD	1:B:73:LYS:CE	2.04	1.35
1:A:92:GLN:OE1	1:A:92:GLN:CD	1.65	1.34
1:B:92:GLN:OE1	1:B:92:GLN:CD	1.65	1.34
1:A:86:LYS:NZ	1:B:103:SER:CB	1.91	1.32
1:A:48:TYR:HE2	2:A:104:HEC:O2D	1.09	1.30
1:B:48:TYR:HE2	2:B:104:HEC:O2D	1.09	1.30
1:A:86:LYS:CD	1:B:103:SER:HB3	1.61	1.30
1:A:44:GLU:CG	1:A:44:GLU:CB	2.09	1.29
1:B:44:GLU:CB	1:B:44:GLU:CG	2.09	1.29
1:A:46:TYR:CG	1:A:46:TYR:CE1	1.96	1.28
1:B:46:TYR:CG	1:B:46:TYR:CE1	1.96	1.28
1:A:66:GLU:CB	1:A:74:TYR:CE2	2.17	1.27

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:GLU:CB	1:B:74:TYR:CE2	2.17	1.27
1:A:10:PHE:CG	1:A:10:PHE:CE2	1.80	1.26
1:B:10:PHE:CG	1:B:10:PHE:CE2	1.80	1.26
1:A:44:GLU:CG	1:A:44:GLU:CD	2.08	1.21
1:B:44:GLU:CG	1:B:44:GLU:CD	2.08	1.21
1:A:16:GLN:N	1:A:16:GLN:CB	2.06	1.17
1:B:16:GLN:N	1:B:16:GLN:CB	2.06	1.17
1:A:24:GLY:O	1:A:25:LYS:HG2	1.45	1.17
1:B:24:GLY:O	1:B:25:LYS:HG2	1.45	1.17
1:A:86:LYS:HE3	1:B:103:SER:OG	1.45	1.15
1:A:86:LYS:HE2	1:B:103:SER:CA	1.67	1.14
1:A:16:GLN:N	1:A:16:GLN:HB3	1.62	1.14
1:A:57:ILE:HD12	1:A:58:VAL:H	1.04	1.14
1:B:16:GLN:N	1:B:16:GLN:HB3	1.62	1.14
1:B:57:ILE:HD12	1:B:58:VAL:H	1.04	1.14
1:A:10:PHE:CD2	1:A:10:PHE:CD1	2.06	1.13
1:B:10:PHE:CD2	1:B:10:PHE:CD1	2.06	1.13
1:A:3:VAL:CA	1:A:3:VAL:CG2	2.25	1.13
1:A:59:TRP:CE3	1:A:63:THR:HG21	1.81	1.13
1:B:3:VAL:CA	1:B:3:VAL:CG2	2.25	1.13
1:B:59:TRP:CE3	1:B:63:THR:HG21	1.81	1.13
2:A:104:HEC:HMC1	2:A:104:HEC:HBC3	1.25	1.13
2:B:104:HEC:HBC3	2:B:104:HEC:HMC1	1.25	1.13
1:A:86:LYS:CE	1:B:103:SER:OG	1.97	1.12
1:A:11:VAL:HA	1:A:15:ALA:HB2	1.16	1.12
1:B:11:VAL:HA	1:B:15:ALA:HB2	1.16	1.12
1:A:26:HIS:O	1:A:27:LYS:CG	1.98	1.11
1:B:26:HIS:O	1:B:27:LYS:CG	1.98	1.11
1:A:86:LYS:HZ3	1:B:102:THR:HG22	1.15	1.11
1:A:47:SER:O	1:A:48:TYR:CB	1.99	1.10
1:B:47:SER:O	1:B:48:TYR:CB	1.99	1.10
1:A:59:TRP:HZ3	1:A:63:THR:HG23	1.10	1.10
1:B:59:TRP:HZ3	1:B:63:THR:HG23	1.10	1.10
1:A:10:PHE:CD2	1:A:10:PHE:CB	2.33	1.10
1:B:10:PHE:CD2	1:B:10:PHE:CB	2.33	1.10
1:A:67:TYR:O	1:A:68:LEU:C	1.80	1.09
1:B:67:TYR:O	1:B:68:LEU:C	1.80	1.09
1:A:59:TRP:CZ3	1:A:63:THR:HG23	1.89	1.07
1:A:86:LYS:NZ	1:B:102:THR:HG22	1.67	1.07
1:B:59:TRP:CZ3	1:B:63:THR:HG23	1.89	1.07
1:A:73:LYS:H	1:A:76:PRO:HB3	1.21	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:LYS:H	1:B:76:PRO:HB3	1.21	1.06
1:A:34:GLY:HA2	1:A:102:THR:HG23	1.32	1.06
1:B:34:GLY:HA2	1:B:102:THR:HG23	1.32	1.06
1:A:59:TRP:CZ3	1:A:63:THR:CG2	2.38	1.05
1:B:59:TRP:CZ3	1:B:63:THR:CG2	2.38	1.05
1:A:36:PHE:N	1:A:36:PHE:HD2	1.55	1.05
1:B:36:PHE:HD2	1:B:36:PHE:N	1.55	1.05
1:A:26:HIS:CG	1:A:26:HIS:CA	2.38	1.05
1:B:26:HIS:CG	1:B:26:HIS:CA	2.38	1.05
1:A:59:TRP:CE3	1:A:63:THR:CG2	2.40	1.04
1:B:59:TRP:CE3	1:B:63:THR:CG2	2.40	1.04
1:A:50:ASP:HB3	1:A:54:SER:OG	1.59	1.03
1:B:50:ASP:HB3	1:B:54:SER:OG	1.59	1.03
1:A:40:THR:CG2	1:A:57:ILE:HG12	1.88	1.03
1:A:57:ILE:CD1	1:A:58:VAL:H	1.70	1.03
1:A:80:MET:HB2	2:A:104:HEC:CHD	1.89	1.03
1:B:40:THR:CG2	1:B:57:ILE:HG12	1.88	1.03
1:B:57:ILE:CD1	1:B:58:VAL:H	1.70	1.03
1:B:80:MET:HB2	2:B:104:HEC:CHD	1.89	1.03
1:A:24:GLY:O	1:A:25:LYS:CG	2.08	1.02
1:B:24:GLY:O	1:B:25:LYS:CG	2.08	1.02
2:A:104:HEC:CMD	2:A:104:HEC:HBD1	1.81	1.01
2:B:104:HEC:CMD	2:B:104:HEC:HBD1	1.81	1.01
1:A:86:LYS:NZ	1:B:103:SER:HB3	1.58	1.01
1:A:70:ASN:HD21	1:A:72:LYS:HB2	1.26	1.00
1:B:70:ASN:HD21	1:B:72:LYS:HB2	1.26	1.00
1:A:47:SER:O	1:A:48:TYR:HB3	1.18	1.00
1:B:47:SER:O	1:B:48:TYR:HB3	1.18	1.00
1:A:74:TYR:H	1:A:76:PRO:HD3	1.26	0.98
1:B:74:TYR:H	1:B:76:PRO:HD3	1.26	0.98
1:A:66:GLU:CB	1:A:74:TYR:CZ	2.43	0.98
1:A:85:ILE:HG22	1:A:85:ILE:O	1.61	0.98
2:A:104:HEC:HMD1	2:A:104:HEC:CBD	1.87	0.98
1:B:66:GLU:CB	1:B:74:TYR:CZ	2.43	0.98
1:B:85:ILE:HG22	1:B:85:ILE:O	1.61	0.98
2:B:104:HEC:HMD1	2:B:104:HEC:CBD	1.87	0.98
1:A:16:GLN:HB3	1:A:16:GLN:H	1.28	0.98
1:B:16:GLN:HB3	1:B:16:GLN:H	1.28	0.98
1:A:72:LYS:O	1:A:73:LYS:HB2	1.61	0.98
1:B:72:LYS:O	1:B:73:LYS:HB2	1.61	0.98
1:A:86:LYS:HE2	1:B:103:SER:HA	1.46	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:MET:HB2	2:A:104:HEC:C1D	1.94	0.96
1:B:80:MET:HB2	2:B:104:HEC:C1D	1.94	0.96
1:A:3:VAL:CA	1:A:3:VAL:CG1	2.43	0.96
1:B:3:VAL:CA	1:B:3:VAL:CG1	2.43	0.96
1:A:48:TYR:CE1	1:A:51:ALA:HB3	2.01	0.96
1:B:48:TYR:CE1	1:B:51:ALA:HB3	2.01	0.96
1:A:68:LEU:HD21	1:A:94:LEU:HG	1.44	0.95
1:B:68:LEU:HD21	1:B:94:LEU:HG	1.44	0.95
1:A:11:VAL:CA	1:A:15:ALA:HB2	1.97	0.95
1:B:11:VAL:CA	1:B:15:ALA:HB2	1.97	0.95
2:A:104:HEC:HBD1	2:A:104:HEC:HMD1	0.97	0.95
2:B:104:HEC:HBD1	2:B:104:HEC:HMD1	0.97	0.95
1:A:56:GLY:O	1:A:57:ILE:HG22	1.67	0.94
1:B:56:GLY:O	1:B:57:ILE:HG22	1.67	0.94
1:A:3:VAL:CA	1:A:3:VAL:HG22	1.96	0.94
1:B:3:VAL:CA	1:B:3:VAL:HG22	1.96	0.94
1:A:50:ASP:O	1:A:51:ALA:CB	2.15	0.94
1:B:50:ASP:O	1:B:51:ALA:CB	2.15	0.94
1:A:3:VAL:CA	1:A:3:VAL:HG23	1.96	0.94
1:A:44:GLU:CB	1:A:44:GLU:CD	2.35	0.94
1:A:66:GLU:HB3	1:A:74:TYR:HE2	1.18	0.94
1:B:3:VAL:CA	1:B:3:VAL:HG23	1.96	0.94
1:B:44:GLU:CB	1:B:44:GLU:CD	2.35	0.94
1:B:66:GLU:HB3	1:B:74:TYR:HE2	1.18	0.94
1:A:46:TYR:CD1	1:A:46:TYR:HB2	2.02	0.93
1:B:46:TYR:CD1	1:B:46:TYR:HB2	2.02	0.93
1:A:35:LEU:HD12	1:A:64:LEU:HD21	1.49	0.93
1:B:35:LEU:HD12	1:B:64:LEU:HD21	1.49	0.93
1:A:10:PHE:CG	1:A:10:PHE:CD2	0.93	0.92
1:B:10:PHE:CG	1:B:10:PHE:CD2	0.93	0.92
1:A:11:VAL:HA	1:A:15:ALA:CB	1.99	0.92
1:B:11:VAL:HA	1:B:15:ALA:CB	1.99	0.92
1:A:26:HIS:O	1:A:27:LYS:HG2	1.68	0.92
1:B:26:HIS:O	1:B:27:LYS:HG2	1.68	0.92
1:A:24:GLY:C	1:A:25:LYS:HG2	1.90	0.91
1:B:24:GLY:C	1:B:25:LYS:HG2	1.90	0.91
1:A:28:VAL:CG1	1:A:29:GLY:N	2.34	0.91
1:B:28:VAL:CG1	1:B:29:GLY:N	2.34	0.91
1:A:46:TYR:CD1	1:A:46:TYR:CG	0.90	0.90
1:A:84:GLY:O	1:A:85:ILE:HB	1.71	0.90
1:B:46:TYR:CD1	1:B:46:TYR:CG	0.90	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:GLY:O	1:B:85:ILE:HB	1.71	0.90
1:A:57:ILE:HD12	1:A:58:VAL:N	1.85	0.90
1:B:57:ILE:HD12	1:B:58:VAL:N	1.85	0.90
1:A:73:LYS:O	1:A:74:TYR:HB2	1.72	0.89
1:A:81:ILE:C	1:A:82:PHE:CA	2.40	0.89
1:B:73:LYS:O	1:B:74:TYR:HB2	1.72	0.89
1:B:81:ILE:C	1:B:82:PHE:CA	2.40	0.89
1:A:70:ASN:ND2	1:A:72:LYS:HB2	1.87	0.89
1:B:70:ASN:ND2	1:B:72:LYS:HB2	1.87	0.89
1:A:40:THR:HG21	1:A:57:ILE:HG12	1.51	0.89
1:B:40:THR:HG21	1:B:57:ILE:HG12	1.51	0.89
1:A:28:VAL:HG12	1:A:29:GLY:H	1.36	0.88
1:A:63:THR:HA	1:A:66:GLU:HB2	1.56	0.88
1:B:28:VAL:HG12	1:B:29:GLY:H	1.36	0.88
1:B:63:THR:HA	1:B:66:GLU:HB2	1.56	0.88
1:A:24:GLY:O	1:A:25:LYS:CB	2.21	0.88
1:A:82:PHE:N	1:A:82:PHE:CB	2.36	0.88
1:B:24:GLY:O	1:B:25:LYS:CB	2.21	0.88
1:B:82:PHE:N	1:B:82:PHE:CB	2.36	0.88
1:A:15:ALA:C	1:A:16:GLN:CA	2.42	0.87
1:B:15:ALA:C	1:B:16:GLN:CA	2.42	0.87
1:A:26:HIS:O	1:A:27:LYS:CB	2.23	0.87
1:B:26:HIS:O	1:B:27:LYS:CB	2.23	0.87
1:A:32:LEU:HD11	2:A:104:HEC:C3A	2.05	0.87
1:B:32:LEU:HD11	2:B:104:HEC:C3A	2.05	0.87
1:A:48:TYR:OH	1:A:78:THR:HA	1.74	0.86
1:A:64:LEU:O	1:A:68:LEU:HB2	1.76	0.86
1:B:48:TYR:OH	1:B:78:THR:HA	1.74	0.86
1:B:64:LEU:O	1:B:68:LEU:HB2	1.76	0.86
1:A:86:LYS:NZ	1:B:103:SER:N	2.24	0.85
2:A:104:HEC:HBC3	2:A:104:HEC:CMC	2.07	0.85
2:B:104:HEC:HBC3	2:B:104:HEC:CMC	2.07	0.85
1:A:59:TRP:CZ3	1:A:63:THR:HG21	2.09	0.85
1:B:59:TRP:CZ3	1:B:63:THR:HG21	2.09	0.85
1:A:16:GLN:H	1:A:16:GLN:HE21	1.25	0.84
1:B:16:GLN:H	1:B:16:GLN:HE21	1.25	0.84
1:A:46:TYR:CG	1:A:46:TYR:HD1	1.58	0.84
1:B:46:TYR:CG	1:B:46:TYR:HD1	1.58	0.84
1:A:59:TRP:HE3	1:A:63:THR:HG21	1.39	0.84
1:A:86:LYS:NZ	1:B:103:SER:OG	2.04	0.84
1:B:59:TRP:HE3	1:B:63:THR:HG21	1.39	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:THR:HG23	1:A:27:LYS:HE3	1.59	0.83
1:B:19:THR:HG23	1:B:27:LYS:HE3	1.59	0.83
1:A:40:THR:CG2	1:A:57:ILE:CG1	2.55	0.83
1:B:40:THR:CG2	1:B:57:ILE:CG1	2.55	0.83
1:A:36:PHE:N	1:A:36:PHE:CD2	2.36	0.83
1:B:36:PHE:N	1:B:36:PHE:CD2	2.36	0.83
1:A:62:ASN:N	1:A:62:ASN:CB	2.41	0.83
1:B:62:ASN:N	1:B:62:ASN:CB	2.41	0.83
1:A:10:PHE:CG	1:A:10:PHE:HD2	1.59	0.83
1:A:17:CYS:C	1:A:18:HIS:CA	2.48	0.83
1:B:10:PHE:CG	1:B:10:PHE:HD2	1.59	0.83
1:B:17:CYS:C	1:B:18:HIS:CA	2.48	0.83
1:A:60:ASN:O	1:A:61:GLU:C	2.17	0.82
1:B:60:ASN:O	1:B:61:GLU:C	2.17	0.82
1:A:56:GLY:O	1:A:57:ILE:CG2	2.27	0.82
1:B:56:GLY:O	1:B:57:ILE:CG2	2.27	0.82
1:A:66:GLU:CG	1:A:74:TYR:HE2	1.93	0.81
1:B:66:GLU:CG	1:B:74:TYR:HE2	1.93	0.81
1:A:19:THR:O	1:A:20:VAL:HB	1.78	0.81
1:B:19:THR:O	1:B:20:VAL:HB	1.78	0.81
1:A:49:THR:CA	1:A:49:THR:CG2	2.55	0.81
1:A:74:TYR:N	1:A:76:PRO:HD3	1.96	0.81
1:B:49:THR:CA	1:B:49:THR:CG2	2.55	0.81
1:B:74:TYR:N	1:B:76:PRO:HD3	1.96	0.81
1:A:101:ALA:N	1:A:101:ALA:CB	2.44	0.81
1:B:101:ALA:N	1:B:101:ALA:CB	2.44	0.81
1:A:43:ALA:O	1:A:44:GLU:CB	2.29	0.80
1:B:43:ALA:O	1:B:44:GLU:CB	2.29	0.80
1:A:69:GLU:O	1:A:70:ASN:HB3	1.80	0.80
1:B:69:GLU:O	1:B:70:ASN:HB3	1.80	0.80
1:A:59:TRP:CE3	1:A:59:TRP:HA	2.17	0.80
1:B:59:TRP:CE3	1:B:59:TRP:HA	2.17	0.80
1:A:34:GLY:O	1:A:35:LEU:C	2.18	0.80
1:B:34:GLY:O	1:B:35:LEU:C	2.18	0.80
1:A:92:GLN:OE1	1:A:92:GLN:CG	2.30	0.80
1:B:92:GLN:OE1	1:B:92:GLN:CG	2.30	0.80
1:A:3:VAL:C	1:A:3:VAL:HG12	2.03	0.80
1:A:48:TYR:CE1	1:A:51:ALA:CB	2.65	0.80
1:B:3:VAL:C	1:B:3:VAL:HG12	2.03	0.80
1:B:48:TYR:CE1	1:B:51:ALA:CB	2.65	0.80
1:A:80:MET:CG	1:A:80:MET:CE	2.60	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:MET:CG	1:B:80:MET:CE	2.60	0.79
1:A:27:LYS:O	1:A:28:VAL:HB	1.75	0.79
1:B:27:LYS:O	1:B:28:VAL:HB	1.75	0.79
1:A:44:GLU:OE2	1:A:44:GLU:HB2	1.83	0.79
1:B:44:GLU:HB2	1:B:44:GLU:OE2	1.83	0.79
1:A:86:LYS:HE2	1:B:103:SER:CB	1.27	0.79
1:A:24:GLY:O	1:A:25:LYS:HB3	1.82	0.79
1:B:24:GLY:O	1:B:25:LYS:HB3	1.82	0.79
1:A:34:GLY:HA2	1:A:102:THR:CG2	2.15	0.77
1:B:34:GLY:HA2	1:B:102:THR:CG2	2.15	0.77
1:A:28:VAL:HG12	1:A:29:GLY:N	1.92	0.77
1:B:28:VAL:HG12	1:B:29:GLY:N	1.92	0.77
1:A:7:LYS:HB2	1:A:97:TYR:CE2	2.20	0.76
1:B:7:LYS:HB2	1:B:97:TYR:CE2	2.20	0.76
1:A:47:SER:OG	1:A:47:SER:CA	2.33	0.76
1:B:47:SER:OG	1:B:47:SER:CA	2.33	0.76
1:A:23:GLY:O	1:A:25:LYS:N	2.18	0.76
1:B:23:GLY:O	1:B:25:LYS:N	2.18	0.76
1:A:50:ASP:CA	1:A:54:SER:HB2	2.15	0.75
1:B:50:ASP:CA	1:B:54:SER:HB2	2.15	0.75
1:A:50:ASP:HB3	1:A:54:SER:CB	2.16	0.75
1:A:86:LYS:NZ	1:B:103:SER:CA	2.43	0.75
1:B:50:ASP:HB3	1:B:54:SER:CB	2.16	0.75
1:A:84:GLY:O	1:A:85:ILE:CB	2.32	0.74
1:B:84:GLY:O	1:B:85:ILE:CB	2.32	0.74
1:A:57:ILE:CG1	1:A:58:VAL:N	2.50	0.74
1:B:57:ILE:CG1	1:B:58:VAL:N	2.50	0.74
1:A:16:GLN:H	1:A:16:GLN:NE2	1.85	0.74
1:A:18:HIS:N	1:A:18:HIS:CB	2.50	0.74
1:B:16:GLN:H	1:B:16:GLN:NE2	1.85	0.74
1:B:18:HIS:N	1:B:18:HIS:CB	2.50	0.74
1:A:3:VAL:CA	1:A:3:VAL:HG12	2.17	0.73
1:B:3:VAL:CA	1:B:3:VAL:HG12	2.17	0.73
1:A:68:LEU:CD2	1:A:94:LEU:HG	2.18	0.73
1:B:68:LEU:CD2	1:B:94:LEU:HG	2.18	0.73
1:A:20:VAL:O	1:A:20:VAL:HG13	1.82	0.73
1:B:20:VAL:O	1:B:20:VAL:HG13	1.82	0.73
1:A:3:VAL:CA	1:A:3:VAL:HG13	2.17	0.73
1:B:3:VAL:CA	1:B:3:VAL:HG13	2.17	0.73
1:A:90:GLU:C	1:A:91:ARG:CA	2.53	0.72
1:B:90:GLU:C	1:B:91:ARG:CA	2.53	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:THR:O	1:A:20:VAL:CB	2.33	0.72
1:B:19:THR:O	1:B:20:VAL:CB	2.33	0.72
1:A:86:LYS:HZ3	1:B:103:SER:N	1.87	0.72
1:A:40:THR:HG23	1:A:57:ILE:CG1	2.19	0.72
1:B:40:THR:HG23	1:B:57:ILE:CG1	2.19	0.72
1:A:26:HIS:CE1	1:A:31:ASN:H	2.06	0.72
1:A:32:LEU:N	1:A:32:LEU:C	2.42	0.72
1:B:26:HIS:CE1	1:B:31:ASN:H	2.06	0.72
1:B:32:LEU:N	1:B:32:LEU:C	2.42	0.72
1:A:86:LYS:HE3	1:B:103:SER:HB2	0.72	0.72
1:A:66:GLU:CB	1:A:74:TYR:OH	2.37	0.72
1:B:66:GLU:CB	1:B:74:TYR:OH	2.37	0.72
1:A:79:LYS:HG3	1:A:79:LYS:O	1.87	0.71
1:B:79:LYS:O	1:B:79:LYS:HG3	1.87	0.71
1:A:59:TRP:HE3	1:A:63:THR:CG2	1.94	0.71
1:A:86:LYS:CD	1:B:103:SER:CB	2.39	0.71
1:B:59:TRP:HE3	1:B:63:THR:CG2	1.94	0.71
1:A:38:ARG:HH12	1:A:43:ALA:HB2	1.56	0.71
1:A:68:LEU:O	1:A:69:GLU:C	2.28	0.71
1:B:38:ARG:HH12	1:B:43:ALA:HB2	1.56	0.71
1:B:68:LEU:O	1:B:69:GLU:C	2.28	0.71
1:A:72:LYS:O	1:A:73:LYS:CB	2.35	0.71
1:B:72:LYS:O	1:B:73:LYS:CB	2.35	0.71
1:A:40:THR:HG23	1:A:57:ILE:HG12	1.72	0.71
1:B:40:THR:HG23	1:B:57:ILE:HG12	1.72	0.71
1:A:24:GLY:C	1:A:25:LYS:CG	2.58	0.70
1:B:24:GLY:C	1:B:25:LYS:CG	2.58	0.70
1:A:57:ILE:O	1:A:58:VAL:HB	1.91	0.70
1:A:87:LYS:O	1:A:88:LYS:C	2.30	0.70
1:B:57:ILE:O	1:B:58:VAL:HB	1.91	0.70
1:B:87:LYS:O	1:B:88:LYS:C	2.30	0.70
1:A:53:LYS:CD	1:A:53:LYS:NZ	2.50	0.70
1:B:53:LYS:CD	1:B:53:LYS:NZ	2.50	0.70
1:A:59:TRP:HZ3	1:A:63:THR:CG2	1.83	0.70
1:B:59:TRP:HZ3	1:B:63:THR:CG2	1.83	0.70
1:A:86:LYS:HE2	1:B:103:SER:HB3	1.04	0.69
1:A:57:ILE:CD1	1:A:58:VAL:N	2.48	0.69
1:B:57:ILE:CD1	1:B:58:VAL:N	2.48	0.69
1:A:3:VAL:HG22	1:A:3:VAL:HA	1.74	0.69
1:B:3:VAL:HG22	1:B:3:VAL:HA	1.74	0.69
1:A:26:HIS:O	1:A:27:LYS:HG3	1.90	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:LEU:HB2	1:A:36:PHE:CE2	2.28	0.69
1:A:48:TYR:OH	1:A:51:ALA:HB1	1.93	0.69
1:B:26:HIS:O	1:B:27:LYS:HG3	1.90	0.69
1:B:35:LEU:HB2	1:B:36:PHE:CE2	2.28	0.69
1:B:48:TYR:OH	1:B:51:ALA:HB1	1.93	0.69
1:A:3:VAL:O	1:A:4:ALA:C	2.29	0.69
1:A:50:ASP:HB3	1:A:54:SER:HG	1.55	0.69
1:B:3:VAL:O	1:B:4:ALA:C	2.29	0.69
1:B:50:ASP:HB3	1:B:54:SER:HG	1.55	0.69
1:A:56:GLY:C	1:A:57:ILE:CG2	2.60	0.68
1:B:56:GLY:C	1:B:57:ILE:CG2	2.60	0.68
1:A:98:LEU:N	1:A:98:LEU:CB	2.55	0.68
1:B:98:LEU:N	1:B:98:LEU:CB	2.55	0.68
1:A:85:ILE:O	1:A:85:ILE:CG2	2.39	0.68
1:B:85:ILE:O	1:B:85:ILE:CG2	2.39	0.68
1:A:32:LEU:HD13	1:A:35:LEU:HD21	1.75	0.68
1:A:66:GLU:HB3	1:A:74:TYR:OH	1.91	0.68
1:B:32:LEU:HD13	1:B:35:LEU:HD21	1.75	0.68
1:B:66:GLU:HB3	1:B:74:TYR:OH	1.91	0.68
1:A:33:TRP:N	1:A:33:TRP:HA	1.98	0.68
1:A:38:ARG:NH1	1:A:43:ALA:HB2	2.09	0.68
1:A:53:LYS:CE	1:A:53:LYS:CG	2.70	0.68
1:B:33:TRP:N	1:B:33:TRP:HA	1.98	0.68
1:B:38:ARG:NH1	1:B:43:ALA:HB2	2.09	0.68
1:B:53:LYS:CE	1:B:53:LYS:CG	2.70	0.68
1:A:44:GLU:CB	1:A:44:GLU:OE2	2.40	0.67
1:B:44:GLU:CB	1:B:44:GLU:OE2	2.40	0.67
1:A:64:LEU:CA	1:A:64:LEU:HD12	2.24	0.67
1:B:64:LEU:CA	1:B:64:LEU:HD12	2.24	0.67
1:A:86:LYS:HE3	1:B:103:SER:CB	0.43	0.67
1:A:14:CYS:SG	2:A:104:HEC:HMB1	2.35	0.67
1:B:14:CYS:SG	2:B:104:HEC:HMB1	2.35	0.67
1:A:36:PHE:HD2	1:A:36:PHE:H	1.34	0.67
1:A:57:ILE:HG13	1:A:58:VAL:N	2.10	0.67
1:B:36:PHE:HD2	1:B:36:PHE:H	1.34	0.67
1:B:57:ILE:HG13	1:B:58:VAL:N	2.10	0.67
1:A:34:GLY:O	1:A:36:PHE:N	2.28	0.67
1:A:66:GLU:CD	1:A:74:TYR:HE2	1.99	0.67
1:B:34:GLY:O	1:B:36:PHE:N	2.28	0.67
1:B:66:GLU:CD	1:B:74:TYR:HE2	1.99	0.67
1:A:61:GLU:C	1:A:62:ASN:CA	2.57	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:GLU:C	1:B:62:ASN:CA	2.57	0.66
1:A:7:LYS:O	1:A:11:VAL:N	2.27	0.66
1:B:7:LYS:O	1:B:11:VAL:N	2.27	0.66
1:A:7:LYS:HB2	1:A:97:TYR:HE2	1.58	0.66
1:A:86:LYS:CE	1:B:103:SER:HB2	1.39	0.66
1:B:7:LYS:HB2	1:B:97:TYR:HE2	1.58	0.66
1:A:86:LYS:CE	1:B:103:SER:CB	0.77	0.66
1:A:66:GLU:CB	1:A:74:TYR:HE2	1.81	0.66
1:B:66:GLU:CB	1:B:74:TYR:HE2	1.81	0.66
1:A:64:LEU:CA	1:A:64:LEU:CG	2.70	0.66
1:A:69:GLU:O	1:A:70:ASN:CB	2.37	0.66
1:B:64:LEU:CA	1:B:64:LEU:CG	2.70	0.66
1:B:69:GLU:O	1:B:70:ASN:CB	2.37	0.66
1:A:100:SER:C	1:A:101:ALA:CA	2.60	0.66
1:B:100:SER:C	1:B:101:ALA:CA	2.60	0.66
1:A:44:GLU:CD	1:A:44:GLU:HB2	2.17	0.65
1:B:44:GLU:CD	1:B:44:GLU:HB2	2.17	0.65
1:A:55:LYS:C	1:A:56:GLY:CA	2.54	0.65
1:A:86:LYS:HZ3	1:B:102:THR:CG2	2.02	0.65
1:B:55:LYS:C	1:B:56:GLY:CA	2.54	0.65
1:A:50:ASP:O	1:A:51:ALA:HB2	1.96	0.65
1:A:63:THR:HG22	1:A:64:LEU:N	2.11	0.65
1:B:50:ASP:O	1:B:51:ALA:HB2	1.96	0.65
1:B:63:THR:HG22	1:B:64:LEU:N	2.11	0.65
1:A:73:LYS:N	1:A:76:PRO:HB3	2.04	0.65
1:B:73:LYS:N	1:B:76:PRO:HB3	2.04	0.65
1:A:26:HIS:CB	1:A:26:HIS:CD2	2.64	0.65
1:B:26:HIS:CB	1:B:26:HIS:CD2	2.64	0.65
1:A:3:VAL:C	1:A:3:VAL:CG1	2.65	0.65
1:A:73:LYS:O	1:A:74:TYR:CB	2.43	0.65
1:B:3:VAL:C	1:B:3:VAL:CG1	2.65	0.65
1:B:73:LYS:O	1:B:74:TYR:CB	2.43	0.65
1:A:7:LYS:CA	1:A:97:TYR:CE2	2.80	0.64
1:B:7:LYS:CA	1:B:97:TYR:CE2	2.80	0.64
1:A:54:SER:O	1:A:56:GLY:N	2.30	0.64
1:A:64:LEU:HD12	1:A:64:LEU:HA	1.80	0.64
1:B:54:SER:O	1:B:56:GLY:N	2.30	0.64
1:B:64:LEU:HD12	1:B:64:LEU:HA	1.80	0.64
1:A:28:VAL:HG13	1:A:29:GLY:N	2.13	0.64
1:B:28:VAL:HG13	1:B:29:GLY:N	2.13	0.64
1:A:50:ASP:HA	1:A:54:SER:HB2	1.77	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:ASP:HA	1:B:54:SER:HB2	1.77	0.64
1:A:91:ARG:N	1:A:91:ARG:C	2.50	0.64
1:B:91:ARG:N	1:B:91:ARG:C	2.50	0.64
1:A:26:HIS:C	1:A:27:LYS:HG3	2.18	0.64
1:B:26:HIS:C	1:B:27:LYS:HG3	2.18	0.64
1:A:31:ASN:C	1:A:32:LEU:CA	2.57	0.63
1:A:67:TYR:O	1:A:68:LEU:O	2.15	0.63
1:B:31:ASN:C	1:B:32:LEU:CA	2.57	0.63
1:B:67:TYR:O	1:B:68:LEU:O	2.15	0.63
1:A:91:ARG:C	1:A:92:GLN:CA	2.60	0.63
1:B:91:ARG:C	1:B:92:GLN:CA	2.60	0.63
1:A:17:CYS:CB	1:A:17:CYS:N	2.59	0.63
1:B:17:CYS:CB	1:B:17:CYS:N	2.59	0.63
1:A:26:HIS:CG	1:A:26:HIS:N	2.66	0.63
1:B:26:HIS:CG	1:B:26:HIS:N	2.66	0.63
1:A:46:TYR:O	1:A:47:SER:CB	2.46	0.63
1:A:48:TYR:CZ	1:A:51:ALA:CB	2.82	0.63
1:B:46:TYR:O	1:B:47:SER:CB	2.46	0.63
1:B:48:TYR:CZ	1:B:51:ALA:CB	2.82	0.63
1:A:50:ASP:O	1:A:51:ALA:HB3	1.99	0.62
1:A:102:THR:HG22	1:A:103:SER:N	2.13	0.62
1:B:50:ASP:O	1:B:51:ALA:HB3	1.99	0.62
1:B:102:THR:HG22	1:B:103:SER:N	2.13	0.62
1:A:83:ALA:CB	1:A:83:ALA:C	2.65	0.62
1:B:83:ALA:CB	1:B:83:ALA:C	2.65	0.62
1:A:41:GLY:O	1:A:42:GLN:C	2.38	0.61
1:B:41:GLY:O	1:B:42:GLN:C	2.38	0.61
1:A:5:LYS:O	1:A:6:GLY:C	2.38	0.61
1:B:5:LYS:O	1:B:6:GLY:C	2.38	0.61
1:A:18:HIS:CE1	1:A:29:GLY:HA3	2.36	0.61
1:B:18:HIS:CE1	1:B:29:GLY:HA3	2.36	0.61
1:A:59:TRP:N	1:A:59:TRP:CB	2.56	0.61
1:A:81:ILE:O	1:A:82:PHE:CA	2.48	0.61
1:B:59:TRP:N	1:B:59:TRP:CB	2.56	0.61
1:B:81:ILE:O	1:B:82:PHE:CA	2.48	0.61
1:A:67:TYR:O	1:A:69:GLU:N	2.30	0.60
1:B:67:TYR:O	1:B:69:GLU:N	2.30	0.60
1:A:60:ASN:CG	1:A:61:GLU:N	2.54	0.60
1:B:60:ASN:CG	1:B:61:GLU:N	2.54	0.60
1:A:43:ALA:N	1:A:43:ALA:C	2.52	0.60
1:A:58:VAL:C	1:A:59:TRP:CA	2.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:ALA:N	1:B:43:ALA:C	2.52	0.60
1:B:58:VAL:C	1:B:59:TRP:CA	2.65	0.60
1:A:3:VAL:HG12	1:A:4:ALA:N	2.16	0.59
1:A:32:LEU:C	1:A:33:TRP:CA	2.53	0.59
1:A:62:ASN:C	1:A:64:LEU:N	2.55	0.59
1:A:68:LEU:HD13	1:A:94:LEU:HB3	1.84	0.59
1:B:3:VAL:HG12	1:B:4:ALA:N	2.16	0.59
1:B:32:LEU:C	1:B:33:TRP:CA	2.53	0.59
1:B:62:ASN:C	1:B:64:LEU:N	2.55	0.59
1:B:68:LEU:HD13	1:B:94:LEU:HB3	1.84	0.59
1:A:48:TYR:CZ	1:A:51:ALA:HB3	2.33	0.59
1:B:48:TYR:CZ	1:B:51:ALA:HB3	2.33	0.59
1:A:42:GLN:C	1:A:43:ALA:CA	2.65	0.59
1:A:64:LEU:CA	1:A:64:LEU:CD1	2.80	0.59
1:B:42:GLN:C	1:B:43:ALA:CA	2.65	0.59
1:B:64:LEU:CA	1:B:64:LEU:CD1	2.80	0.59
1:A:26:HIS:ND1	1:A:31:ASN:N	2.50	0.59
1:B:26:HIS:ND1	1:B:31:ASN:N	2.50	0.59
1:A:3:VAL:CA	1:A:3:VAL:CB	2.81	0.59
1:A:5:LYS:CG	1:A:5:LYS:CE	2.74	0.59
1:B:3:VAL:CA	1:B:3:VAL:CB	2.81	0.59
1:B:5:LYS:CG	1:B:5:LYS:CE	2.74	0.59
1:A:7:LYS:CB	1:A:97:TYR:CE2	2.86	0.58
1:A:66:GLU:HB2	1:A:74:TYR:OH	2.02	0.58
1:B:7:LYS:CB	1:B:97:TYR:CE2	2.86	0.58
1:B:66:GLU:HB2	1:B:74:TYR:OH	2.02	0.58
1:A:57:ILE:CG1	1:A:58:VAL:H	2.13	0.58
1:B:57:ILE:CG1	1:B:58:VAL:H	2.13	0.58
1:A:81:ILE:O	1:A:82:PHE:HA	2.03	0.58
1:B:81:ILE:O	1:B:82:PHE:HA	2.03	0.58
1:A:43:ALA:O	1:A:44:GLU:HB2	2.03	0.58
1:B:43:ALA:O	1:B:44:GLU:HB2	2.03	0.58
1:A:70:ASN:HD21	1:A:72:LYS:CB	2.10	0.58
1:B:70:ASN:HD21	1:B:72:LYS:CB	2.10	0.58
1:A:11:VAL:O	1:A:15:ALA:HB3	2.04	0.58
1:A:48:TYR:OH	1:A:78:THR:CA	2.49	0.58
1:B:11:VAL:O	1:B:15:ALA:HB3	2.04	0.58
1:B:48:TYR:OH	1:B:78:THR:CA	2.49	0.58
1:A:63:THR:CA	1:A:66:GLU:HB2	2.31	0.57
1:B:63:THR:CA	1:B:66:GLU:HB2	2.31	0.57
1:A:38:ARG:O	1:A:59:TRP:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:ARG:O	1:B:59:TRP:N	2.37	0.57
1:A:40:THR:HG23	1:A:57:ILE:HG13	1.85	0.57
1:A:56:GLY:C	1:A:57:ILE:HG23	2.23	0.57
1:B:40:THR:HG23	1:B:57:ILE:HG13	1.85	0.57
1:B:56:GLY:C	1:B:57:ILE:HG23	2.23	0.57
1:A:86:LYS:CD	1:A:86:LYS:NZ	2.67	0.57
1:A:92:GLN:N	1:A:92:GLN:C	2.56	0.57
1:B:86:LYS:CD	1:B:86:LYS:NZ	2.67	0.57
1:B:92:GLN:N	1:B:92:GLN:C	2.56	0.57
1:A:66:GLU:CG	1:A:74:TYR:CE2	2.74	0.56
1:B:66:GLU:CG	1:B:74:TYR:CE2	2.74	0.56
1:A:26:HIS:C	1:A:27:LYS:CG	2.67	0.56
1:B:26:HIS:C	1:B:27:LYS:CG	2.67	0.56
1:A:93:ASP:O	1:A:94:LEU:C	2.40	0.56
1:B:93:ASP:O	1:B:94:LEU:C	2.40	0.56
1:A:11:VAL:CA	1:A:15:ALA:CB	2.72	0.55
1:B:11:VAL:CA	1:B:15:ALA:CB	2.72	0.55
1:A:26:HIS:CA	1:A:26:HIS:ND1	2.70	0.55
1:B:26:HIS:CA	1:B:26:HIS:ND1	2.70	0.55
1:A:47:SER:CB	1:A:47:SER:HG	2.12	0.54
1:B:47:SER:CB	1:B:47:SER:HG	2.12	0.54
1:A:51:ALA:N	1:A:54:SER:HB2	2.23	0.54
1:B:51:ALA:N	1:B:54:SER:HB2	2.23	0.54
1:A:51:ALA:O	1:A:53:LYS:N	2.41	0.54
1:B:51:ALA:O	1:B:53:LYS:N	2.41	0.54
1:A:26:HIS:O	1:A:27:LYS:HB3	2.04	0.54
1:B:26:HIS:O	1:B:27:LYS:HB3	2.04	0.54
1:A:32:LEU:CD1	2:A:104:HEC:HMA3	2.37	0.54
1:B:32:LEU:CD1	2:B:104:HEC:HMA3	2.37	0.54
1:A:59:TRP:HE3	1:A:59:TRP:HA	1.69	0.54
1:B:59:TRP:HE3	1:B:59:TRP:HA	1.69	0.54
1:A:6:GLY:O	1:A:7:LYS:C	2.45	0.54
1:B:6:GLY:O	1:B:7:LYS:C	2.45	0.54
1:A:50:ASP:C	1:A:54:SER:HB2	2.28	0.53
1:A:80:MET:CB	2:A:104:HEC:C1D	2.79	0.53
1:B:50:ASP:C	1:B:54:SER:HB2	2.28	0.53
1:B:80:MET:CB	2:B:104:HEC:C1D	2.79	0.53
1:A:98:LEU:N	1:A:98:LEU:CG	2.71	0.53
1:B:98:LEU:N	1:B:98:LEU:CG	2.71	0.53
1:A:63:THR:CG2	1:A:64:LEU:N	2.60	0.53
1:B:63:THR:CG2	1:B:64:LEU:N	2.60	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:THR:OG1	1:A:74:TYR:OH	2.20	0.53
1:A:86:LYS:CE	1:B:103:SER:HG	2.19	0.53
1:B:63:THR:OG1	1:B:74:TYR:OH	2.20	0.53
1:A:86:LYS:HZ1	1:B:103:SER:H	1.57	0.53
1:A:26:HIS:CG	1:A:30:PRO:HA	2.45	0.52
1:B:26:HIS:CG	1:B:30:PRO:HA	2.45	0.52
1:A:94:LEU:O	1:A:97:TYR:N	2.41	0.52
1:B:94:LEU:O	1:B:97:TYR:N	2.41	0.52
1:A:55:LYS:HZ2	1:A:74:TYR:HA	1.75	0.52
1:B:55:LYS:HZ2	1:B:74:TYR:HA	1.75	0.52
1:A:17:CYS:CB	1:A:17:CYS:C	2.72	0.52
1:B:17:CYS:CB	1:B:17:CYS:C	2.72	0.52
1:A:46:TYR:HB2	1:A:46:TYR:HD1	1.59	0.52
1:B:46:TYR:HB2	1:B:46:TYR:HD1	1.59	0.52
1:A:32:LEU:HD13	1:A:35:LEU:CD2	2.39	0.52
1:A:86:LYS:HZ1	1:B:103:SER:N	2.06	0.52
1:B:32:LEU:HD13	1:B:35:LEU:CD2	2.39	0.52
1:A:91:ARG:N	1:A:91:ARG:CB	2.63	0.52
1:B:91:ARG:N	1:B:91:ARG:CB	2.63	0.52
1:A:46:TYR:O	1:A:47:SER:HB3	2.10	0.52
1:A:86:LYS:CE	1:A:86:LYS:CG	2.86	0.52
1:B:46:TYR:O	1:B:47:SER:HB3	2.10	0.52
1:B:86:LYS:CE	1:B:86:LYS:CG	2.86	0.52
1:A:91:ARG:O	1:A:92:GLN:C	2.49	0.51
1:B:91:ARG:O	1:B:92:GLN:C	2.49	0.51
1:A:30:PRO:O	1:A:31:ASN:C	2.48	0.51
1:A:48:TYR:OH	1:A:51:ALA:CB	2.59	0.51
1:A:50:ASP:HB3	1:A:54:SER:HB2	1.90	0.51
1:B:30:PRO:O	1:B:31:ASN:C	2.48	0.51
1:B:48:TYR:OH	1:B:51:ALA:CB	2.59	0.51
1:B:50:ASP:HB3	1:B:54:SER:HB2	1.90	0.51
1:A:54:SER:O	1:A:55:LYS:C	2.50	0.51
1:B:54:SER:O	1:B:55:LYS:C	2.50	0.51
1:A:32:LEU:CD1	1:A:35:LEU:HD21	2.40	0.50
1:B:32:LEU:CD1	1:B:35:LEU:HD21	2.40	0.50
1:A:3:VAL:HG23	1:A:3:VAL:N	2.26	0.50
1:A:101:ALA:N	1:A:101:ALA:C	2.59	0.50
1:B:3:VAL:HG23	1:B:3:VAL:N	2.26	0.50
1:B:101:ALA:N	1:B:101:ALA:C	2.59	0.50
1:A:70:ASN:ND2	1:A:72:LYS:CB	2.70	0.50
1:B:70:ASN:ND2	1:B:72:LYS:CB	2.70	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:THR:CB	1:A:49:THR:C	2.60	0.50
1:A:96:ALA:O	1:A:97:TYR:C	2.50	0.50
1:B:49:THR:CB	1:B:49:THR:C	2.60	0.50
1:B:96:ALA:O	1:B:97:TYR:C	2.50	0.50
1:A:32:LEU:HD11	2:A:104:HEC:CMA	2.41	0.50
1:B:32:LEU:HD11	2:B:104:HEC:CMA	2.41	0.50
1:A:10:PHE:CD2	1:A:14:CYS:HB2	2.47	0.49
1:B:10:PHE:CD2	1:B:14:CYS:HB2	2.47	0.49
1:A:3:VAL:C	1:A:3:VAL:N	2.61	0.49
1:B:3:VAL:C	1:B:3:VAL:N	2.61	0.49
1:A:19:THR:HG21	1:A:25:LYS:HE2	1.94	0.49
1:B:19:THR:HG21	1:B:25:LYS:HE2	1.94	0.49
1:A:50:ASP:CB	1:A:54:SER:HB2	2.42	0.49
1:B:50:ASP:CB	1:B:54:SER:HB2	2.42	0.49
1:A:17:CYS:O	1:A:18:HIS:CA	2.61	0.49
1:A:24:GLY:N	1:A:24:GLY:C	2.63	0.49
1:B:17:CYS:O	1:B:18:HIS:CA	2.61	0.49
1:B:24:GLY:N	1:B:24:GLY:C	2.63	0.49
1:A:32:LEU:HD11	2:A:104:HEC:C2A	2.43	0.48
1:A:83:ALA:CB	1:A:84:GLY:N	2.75	0.48
1:B:32:LEU:HD11	2:B:104:HEC:C2A	2.43	0.48
1:B:83:ALA:CB	1:B:84:GLY:N	2.75	0.48
1:A:57:ILE:O	1:A:58:VAL:CB	2.51	0.48
1:B:57:ILE:O	1:B:58:VAL:CB	2.51	0.48
1:A:70:ASN:ND2	1:A:70:ASN:C	2.68	0.47
1:A:79:LYS:HE2	2:A:104:HEC:CBD	2.45	0.47
1:B:70:ASN:ND2	1:B:70:ASN:C	2.68	0.47
1:B:79:LYS:HE2	2:B:104:HEC:CBD	2.45	0.47
1:A:49:THR:CA	1:A:49:THR:OG1	2.53	0.47
1:B:49:THR:CA	1:B:49:THR:OG1	2.53	0.47
1:A:48:TYR:OH	1:A:79:LYS:N	2.48	0.47
1:B:48:TYR:OH	1:B:79:LYS:N	2.48	0.47
1:A:9:THR:HG21	1:A:94:LEU:HD22	1.96	0.47
1:B:9:THR:HG21	1:B:94:LEU:HD22	1.96	0.47
1:A:94:LEU:O	1:A:95:VAL:C	2.53	0.46
1:B:94:LEU:O	1:B:95:VAL:C	2.53	0.46
1:A:39:LYS:HA	1:A:58:VAL:HA	1.97	0.46
1:B:39:LYS:HA	1:B:58:VAL:HA	1.97	0.46
1:A:10:PHE:CD2	1:A:14:CYS:CB	2.98	0.46
1:B:10:PHE:CD2	1:B:14:CYS:CB	2.98	0.46
1:A:44:GLU:CD	1:A:44:GLU:HA	2.35	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:GLN:O	1:A:93:ASP:C	2.50	0.46
1:B:44:GLU:CD	1:B:44:GLU:HA	2.35	0.46
1:B:92:GLN:O	1:B:93:ASP:C	2.50	0.46
1:A:86:LYS:CE	1:B:103:SER:HB3	0.21	0.45
1:A:85:ILE:HD12	1:A:94:LEU:HD23	1.97	0.45
1:B:85:ILE:HD12	1:B:94:LEU:HD23	1.97	0.45
1:A:79:LYS:HE2	2:A:104:HEC:HBD1	1.98	0.45
1:B:79:LYS:HE2	2:B:104:HEC:HBD1	1.98	0.45
1:A:25:LYS:O	1:A:26:HIS:O	2.35	0.45
1:A:31:ASN:O	1:A:32:LEU:CA	2.63	0.45
1:B:25:LYS:O	1:B:26:HIS:O	2.35	0.45
1:B:31:ASN:O	1:B:32:LEU:CA	2.63	0.45
1:A:10:PHE:CE2	1:A:14:CYS:HB3	2.52	0.45
1:A:31:ASN:HB3	1:A:33:TRP:CD1	2.51	0.45
1:A:66:GLU:OE2	1:A:74:TYR:CE2	2.69	0.45
1:B:10:PHE:CE2	1:B:14:CYS:HB3	2.52	0.45
1:B:31:ASN:HB3	1:B:33:TRP:CD1	2.51	0.45
1:B:66:GLU:OE2	1:B:74:TYR:CE2	2.69	0.45
1:A:66:GLU:CD	1:A:74:TYR:CE2	2.85	0.45
1:B:66:GLU:CD	1:B:74:TYR:CE2	2.85	0.45
1:A:36:PHE:HE1	1:A:99:LYS:CA	2.31	0.44
1:A:70:ASN:O	1:A:72:LYS:N	2.50	0.44
1:B:36:PHE:HE1	1:B:99:LYS:CA	2.31	0.44
1:B:70:ASN:O	1:B:72:LYS:N	2.50	0.44
1:A:43:ALA:O	1:A:44:GLU:HB3	2.14	0.44
1:A:92:GLN:HG2	1:A:93:ASP:N	2.32	0.44
1:B:43:ALA:O	1:B:44:GLU:HB3	2.14	0.44
1:B:92:GLN:HG2	1:B:93:ASP:N	2.32	0.44
1:A:12:GLN:C	1:A:13:LYS:HG2	2.19	0.44
1:A:53:LYS:O	1:A:56:GLY:N	2.50	0.44
1:B:12:GLN:C	1:B:13:LYS:HG2	2.19	0.44
1:B:53:LYS:O	1:B:56:GLY:N	2.50	0.44
1:A:80:MET:HB2	2:A:104:HEC:C2D	2.41	0.44
1:B:80:MET:HB2	2:B:104:HEC:C2D	2.41	0.44
1:A:9:THR:CG2	1:A:94:LEU:HD22	2.48	0.43
1:A:70:ASN:HA	1:A:71:PRO:HD3	1.66	0.43
1:B:9:THR:CG2	1:B:94:LEU:HD22	2.48	0.43
1:B:70:ASN:HA	1:B:71:PRO:HD3	1.66	0.43
1:A:32:LEU:HD11	2:A:104:HEC:HMA3	2.01	0.43
1:A:32:LEU:CD1	2:A:104:HEC:CMA	2.96	0.43
1:B:32:LEU:HD11	2:B:104:HEC:HMA3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:LEU:CD1	2:B:104:HEC:CMA	2.96	0.43
1:A:15:ALA:O	1:A:16:GLN:CA	2.63	0.43
1:A:44:GLU:OE2	1:A:44:GLU:CA	2.66	0.43
1:B:15:ALA:O	1:B:16:GLN:CA	2.63	0.43
1:B:44:GLU:OE2	1:B:44:GLU:CA	2.66	0.43
1:A:32:LEU:CD2	2:A:104:HEC:HBA1	2.49	0.43
1:A:94:LEU:HA	1:A:94:LEU:HD13	1.54	0.43
1:B:32:LEU:CD2	2:B:104:HEC:HBA1	2.49	0.43
1:B:94:LEU:HA	1:B:94:LEU:HD13	1.54	0.43
1:A:6:GLY:HA3	1:A:97:TYR:HB2	2.00	0.43
1:A:98:LEU:CA	1:A:99:LYS:N	2.64	0.43
1:B:6:GLY:HA3	1:B:97:TYR:HB2	2.00	0.43
1:B:98:LEU:CA	1:B:99:LYS:N	2.64	0.43
1:A:59:TRP:N	1:A:59:TRP:HA	2.07	0.43
1:B:59:TRP:N	1:B:59:TRP:HA	2.07	0.43
1:A:14:CYS:SG	2:A:104:HEC:CMB	3.00	0.43
1:B:14:CYS:SG	2:B:104:HEC:CMB	3.00	0.43
1:A:44:GLU:CD	1:A:44:GLU:CA	2.87	0.43
1:B:44:GLU:CD	1:B:44:GLU:CA	2.87	0.43
1:A:65:MET:HE3	1:A:92:GLN:N	2.34	0.43
1:A:68:LEU:CD1	1:A:94:LEU:HB3	2.48	0.43
1:B:65:MET:HE3	1:B:92:GLN:N	2.34	0.43
1:B:68:LEU:CD1	1:B:94:LEU:HB3	2.48	0.43
1:A:18:HIS:N	1:A:18:HIS:CG	2.87	0.42
1:B:18:HIS:N	1:B:18:HIS:CG	2.87	0.42
1:A:90:GLU:O	1:A:91:ARG:CA	2.66	0.42
1:B:90:GLU:O	1:B:91:ARG:CA	2.66	0.42
1:A:48:TYR:HH	1:A:78:THR:HA	1.80	0.42
1:A:65:MET:O	1:A:66:GLU:C	2.55	0.42
1:B:48:TYR:HH	1:B:78:THR:HA	1.80	0.42
1:B:65:MET:O	1:B:66:GLU:C	2.55	0.42
1:A:98:LEU:C	1:A:98:LEU:N	2.71	0.42
1:B:98:LEU:C	1:B:98:LEU:N	2.71	0.42
1:A:17:CYS:HB3	1:A:18:HIS:H	1.84	0.42
1:A:86:LYS:NZ	1:B:102:THR:CG2	2.59	0.42
1:B:17:CYS:HB3	1:B:18:HIS:H	1.84	0.42
1:A:74:TYR:O	1:A:75:ILE:C	2.56	0.42
1:A:83:ALA:CB	1:A:83:ALA:N	2.71	0.42
1:B:74:TYR:O	1:B:75:ILE:C	2.56	0.42
1:B:83:ALA:CB	1:B:83:ALA:N	2.71	0.42
1:A:21:GLU:HB3	1:A:22:ASN:H	1.72	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:GLU:HB3	1:B:22:ASN:H	1.72	0.41
1:A:38:ARG:HH12	1:A:43:ALA:CB	2.30	0.41
1:A:72:LYS:NZ	1:A:72:LYS:CD	2.72	0.41
1:B:38:ARG:HH12	1:B:43:ALA:CB	2.30	0.41
1:B:72:LYS:NZ	1:B:72:LYS:CD	2.72	0.41
1:A:12:GLN:CG	1:A:12:GLN:OE1	2.69	0.41
1:B:12:GLN:CG	1:B:12:GLN:OE1	2.69	0.41
1:A:53:LYS:O	1:A:54:SER:C	2.59	0.41
1:B:53:LYS:O	1:B:54:SER:C	2.59	0.41
1:A:17:CYS:CB	1:A:18:HIS:N	2.84	0.40
1:A:32:LEU:HD21	2:A:104:HEC:HBA1	2.04	0.40
1:A:91:ARG:C	1:A:92:GLN:C	2.80	0.40
1:B:17:CYS:CB	1:B:18:HIS:N	2.84	0.40
1:B:32:LEU:HD21	2:B:104:HEC:HBA1	2.04	0.40
1:B:91:ARG:C	1:B:92:GLN:C	2.80	0.40
1:A:55:LYS:NZ	1:A:74:TYR:HA	2.37	0.40
1:A:64:LEU:O	1:A:68:LEU:CB	2.57	0.40
1:B:55:LYS:NZ	1:B:74:TYR:HA	2.37	0.40
1:B:64:LEU:O	1:B:68:LEU:CB	2.57	0.40
1:A:59:TRP:HA	1:A:63:THR:HG21	2.04	0.40
1:B:59:TRP:HA	1:B:63:THR:HG21	2.04	0.40

All (54) 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:A:88:LYS:CE	1:B:88:LYS:CD[4_455]	0.41	1.79
1:A:88:LYS:CD	1:B:88:LYS:CE[4_455]	0.41	1.79
1:A:16:GLN:OE1	1:A:47:SER:OG[2_454]	0.69	1.51
1:B:16:GLN:OE1	1:B:47:SER:OG[2_554]	0.69	1.51
1:A:103:SER:CB	1:B:86:LYS:CE[1_455]	0.77	1.43
1:A:55:LYS:O	1:B:62:ASN:CG[4_456]	0.79	1.41
1:A:62:ASN:CG	1:B:55:LYS:O[4_456]	0.79	1.41
1:A:88:LYS:CG	1:B:88:LYS:NZ[4_455]	0.90	1.30
1:A:88:LYS:NZ	1:B:88:LYS:CG[4_455]	0.90	1.30
1:A:55:LYS:O	1:B:62:ASN:ND2[4_456]	0.91	1.29
1:A:62:ASN:ND2	1:B:55:LYS:O[4_456]	0.91	1.29
1:A:55:LYS:C	1:B:62:ASN:ND2[4_456]	0.98	1.22
1:A:62:ASN:ND2	1:B:55:LYS:C[4_456]	0.98	1.22
1:A:88:LYS:CE	1:B:88:LYS:CE[4_455]	1.11	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:LYS:CD	1:B:88:LYS:NZ[4_455]	1.18	1.02
1:A:88:LYS:NZ	1:B:88:LYS:CD[4_455]	1.18	1.02
1:A:88:LYS:CD	1:B:88:LYS:CD[4_455]	1.24	0.96
1:A:92:GLN:CB	1:B:92:GLN:NE2[4_455]	1.27	0.93
1:A:92:GLN:NE2	1:B:92:GLN:CB[4_455]	1.27	0.93
1:A:73:LYS:CE	1:B:73:LYS:NZ[4_456]	1.38	0.82
1:A:73:LYS:NZ	1:B:73:LYS:CE[4_456]	1.38	0.82
1:A:16:GLN:OE1	1:A:47:SER:CB[2_454]	1.43	0.77
1:B:16:GLN:OE1	1:B:47:SER:CB[2_554]	1.43	0.77
1:A:73:LYS:CE	1:B:73:LYS:CE[4_456]	1.53	0.67
1:A:55:LYS:O	1:B:62:ASN:CB[4_456]	1.67	0.53
1:A:62:ASN:CB	1:B:55:LYS:O[4_456]	1.67	0.53
1:A:55:LYS:C	1:B:62:ASN:CG[4_456]	1.68	0.52
1:A:62:ASN:CG	1:B:55:LYS:C[4_456]	1.68	0.52
1:A:16:GLN:CD	1:A:47:SER:OG[2_454]	1.70	0.50
1:B:16:GLN:CD	1:B:47:SER:OG[2_554]	1.70	0.50
1:A:73:LYS:NZ	1:B:73:LYS:NZ[4_456]	1.72	0.48
1:A:88:LYS:CG	1:B:88:LYS:CE[4_455]	1.72	0.48
1:A:88:LYS:CE	1:B:88:LYS:CG[4_455]	1.72	0.48
1:A:58:VAL:CG1	1:B:58:VAL:CG1[4_456]	1.79	0.41
1:A:11:VAL:O	1:A:79:LYS:NZ[2_454]	1.86	0.34
1:B:11:VAL:O	1:B:79:LYS:NZ[2_554]	1.86	0.34
1:A:16:GLN:CG	1:A:47:SER:C[2_454]	1.89	0.31
1:B:16:GLN:CG	1:B:47:SER:C[2_554]	1.89	0.31
1:A:103:SER:CB	1:B:86:LYS:NZ[1_455]	1.91	0.29
1:A:56:GLY:N	1:B:62:ASN:ND2[4_456]	1.94	0.26
1:A:62:ASN:ND2	1:B:56:GLY:N[4_456]	1.94	0.26
1:A:103:SER:OG	1:B:86:LYS:CE[1_455]	1.97	0.23
1:A:103:SER:CA	1:B:86:LYS:CE[1_455]	2.01	0.19
1:A:55:LYS:CA	1:B:62:ASN:ND2[4_456]	2.03	0.17
1:A:62:ASN:ND2	1:B:55:LYS:CA[4_456]	2.03	0.17
1:A:92:GLN:CG	1:B:92:GLN:NE2[4_455]	2.04	0.16
1:A:92:GLN:NE2	1:B:92:GLN:CG[4_455]	2.04	0.16
1:A:103:SER:OG	1:B:86:LYS:NZ[1_455]	2.04	0.16
1:A:16:GLN:CG	1:A:48:TYR:CB[2_454]	2.06	0.14
1:B:16:GLN:CG	1:B:48:TYR:CB[2_554]	2.06	0.14
1:A:88:LYS:CE	1:B:88:LYS:NZ[4_455]	2.10	0.10
1:A:88:LYS:NZ	1:B:88:LYS:CE[4_455]	2.10	0.10
1:A:16:GLN:CB	1:A:48:TYR:CB[2_454]	2.15	0.05
1:B:16:GLN:CB	1:B:48:TYR:CB[2_554]	2.15	0.05

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	101/103 (98%)	42 (42%)	21 (21%)	38 (38%)	0	0
1	B	101/103 (98%)	42 (42%)	21 (21%)	38 (38%)	0	0
All	All	202/206 (98%)	84 (42%)	42 (21%)	76 (38%)	0	0

All (76) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	15	ALA
1	A	18	HIS
1	A	20	VAL
1	A	24	GLY
1	A	25	LYS
1	A	27	LYS
1	A	28	VAL
1	A	30	PRO
1	A	33	TRP
1	A	42	GLN
1	A	44	GLU
1	A	47	SER
1	A	48	TYR
1	A	53	LYS
1	A	55	LYS
1	A	56	GLY
1	A	57	ILE
1	A	62	ASN
1	A	63	THR
1	A	69	GLU
1	A	74	TYR
1	B	15	ALA
1	B	18	HIS
1	B	20	VAL
1	B	24	GLY

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Mol	Chain	Res	Type
1	B	25	LYS
1	B	27	LYS
1	B	28	VAL
1	B	30	PRO
1	B	33	TRP
1	B	42	GLN
1	B	44	GLU
1	B	47	SER
1	B	48	TYR
1	B	53	LYS
1	B	55	LYS
1	B	56	GLY
1	B	57	ILE
1	B	62	ASN
1	B	63	THR
1	B	69	GLU
1	B	74	TYR
1	A	35	LEU
1	A	36	PHE
1	A	51	ALA
1	A	52	ASN
1	A	54	SER
1	A	73	LYS
1	A	85	ILE
1	B	35	LEU
1	B	36	PHE
1	B	51	ALA
1	B	52	ASN
1	B	54	SER
1	B	73	LYS
1	B	85	ILE
1	A	26	HIS
1	A	89	GLY
1	B	26	HIS
1	B	89	GLY
1	A	61	GLU
1	A	88	LYS
1	B	61	GLU
1	B	88	LYS
1	A	83	ALA
1	A	92	GLN
1	B	83	ALA

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Mol	Chain	Res	Type
1	B	92	GLN
1	A	81	ILE
1	A	94	LEU
1	B	81	ILE
1	B	94	LEU
1	A	58	VAL
1	B	58	VAL
1	A	75	ILE
1	B	75	ILE

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	81/83 (98%)	49 (60%)	32 (40%)	0 0
1	B	81/83 (98%)	49 (60%)	32 (40%)	0 0
All	All	162/166 (98%)	98 (60%)	64 (40%)	0 0

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	THR
1	A	11	VAL
1	A	13	LYS
1	A	16	GLN
1	A	17	CYS
1	A	20	VAL
1	A	21	GLU
1	A	27	LYS
1	A	28	VAL
1	A	32	LEU
1	A	33	TRP
1	A	38	ARG
1	A	40	THR
1	A	42	GLN

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Mol	Chain	Res	Type
1	A	46	TYR
1	A	50	ASP
1	A	57	ILE
1	A	61	GLU
1	A	63	THR
1	A	64	LEU
1	A	65	MET
1	A	70	ASN
1	A	75	ILE
1	A	78	THR
1	A	80	MET
1	A	81	ILE
1	A	85	ILE
1	A	86	LYS
1	A	88	LYS
1	A	92	GLN
1	A	94	LEU
1	A	102	THR
1	B	9	THR
1	B	11	VAL
1	B	13	LYS
1	B	16	GLN
1	B	17	CYS
1	B	20	VAL
1	B	21	GLU
1	B	27	LYS
1	B	28	VAL
1	B	32	LEU
1	B	33	TRP
1	B	38	ARG
1	B	40	THR
1	B	42	GLN
1	B	46	TYR
1	B	50	ASP
1	B	57	ILE
1	B	61	GLU
1	B	63	THR
1	B	64	LEU
1	B	65	MET
1	B	70	ASN
1	B	75	ILE
1	B	78	THR

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Mol	Chain	Res	Type
1	B	80	MET
1	B	81	ILE
1	B	85	ILE
1	B	86	LYS
1	B	88	LYS
1	B	92	GLN
1	B	94	LEU
1	B	102	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	16	GLN
1	A	31	ASN
1	A	42	GLN
1	A	52	ASN
1	A	70	ASN
1	B	12	GLN
1	B	16	GLN
1	B	31	ASN
1	B	42	GLN
1	B	52	ASN
1	B	70	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

2 ligands 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	HEC	B	104	1	26,50,50	7.07	19 (73%)	18,82,82	5.79	10 (55%)
2	HEC	A	104	1	26,50,50	7.07	19 (73%)	18,82,82	5.79	10 (55%)

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	HEC	B	104	1	-	4/6/54/54	-
2	HEC	A	104	1	-	4/6/54/54	-

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	104	HEC	C3C-C2C	-18.47	1.21	1.40
2	B	104	HEC	C3C-C2C	-18.47	1.21	1.40
2	A	104	HEC	C3B-C4B	-14.84	1.16	1.43
2	B	104	HEC	C3B-C4B	-14.84	1.16	1.43
2	A	104	HEC	CAA-C2A	-14.70	1.26	1.52
2	B	104	HEC	CAA-C2A	-14.70	1.26	1.52
2	A	104	HEC	CMD-C2D	-9.44	1.32	1.51
2	B	104	HEC	CMD-C2D	-9.44	1.32	1.51
2	A	104	HEC	C1B-NB	-9.41	1.16	1.36
2	B	104	HEC	C1B-NB	-9.41	1.16	1.36
2	A	104	HEC	C1C-CHC	-8.52	1.17	1.41
2	B	104	HEC	C1C-CHC	-8.52	1.17	1.41
2	A	104	HEC	C4A-C3A	-7.57	1.25	1.42
2	B	104	HEC	C4A-C3A	-7.57	1.25	1.42
2	A	104	HEC	C1A-C2A	-6.84	1.27	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	104	HEC	C1A-C2A	-6.84	1.27	1.42
2	A	104	HEC	C1C-NC	5.97	1.48	1.36
2	B	104	HEC	C1C-NC	5.97	1.48	1.36
2	A	104	HEC	C2A-C3A	5.25	1.53	1.37
2	B	104	HEC	C2A-C3A	5.25	1.53	1.37
2	A	104	HEC	CBC-CAC	-5.10	1.30	1.49
2	B	104	HEC	CBC-CAC	-5.10	1.30	1.49
2	A	104	HEC	CBB-CAB	-3.40	1.36	1.49
2	B	104	HEC	CBB-CAB	-3.40	1.36	1.49
2	A	104	HEC	C3B-C2B	3.35	1.44	1.40
2	B	104	HEC	C3B-C2B	3.35	1.44	1.40
2	A	104	HEC	CMB-C2B	-3.30	1.43	1.51
2	B	104	HEC	CMB-C2B	-3.30	1.43	1.51
2	A	104	HEC	CBD-CAD	-3.08	1.32	1.53
2	B	104	HEC	CBD-CAD	-3.08	1.32	1.53
2	A	104	HEC	C1D-ND	2.85	1.42	1.36
2	B	104	HEC	C1D-ND	2.85	1.42	1.36
2	A	104	HEC	C3C-C4C	2.39	1.47	1.43
2	B	104	HEC	C3C-C4C	2.39	1.47	1.43
2	A	104	HEC	C1D-CHD	-2.16	1.35	1.41
2	B	104	HEC	C1D-CHD	-2.16	1.35	1.41
2	A	104	HEC	C4D-CHA	-2.06	1.35	1.41
2	B	104	HEC	C4D-CHA	-2.06	1.35	1.41

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	104	HEC	C4C-C3C-C2C	16.56	124.23	106.35
2	B	104	HEC	C4C-C3C-C2C	16.56	124.23	106.35
2	A	104	HEC	CAD-CBD-CGD	8.82	127.47	112.67
2	B	104	HEC	CAD-CBD-CGD	8.82	127.47	112.67
2	A	104	HEC	C3C-C4C-NC	-8.03	95.79	110.94
2	B	104	HEC	C3C-C4C-NC	-8.03	95.79	110.94
2	A	104	HEC	C4B-C3B-C2B	-7.90	97.82	106.35
2	B	104	HEC	C4B-C3B-C2B	-7.90	97.82	106.35
2	A	104	HEC	C3B-C4B-NB	6.86	123.90	110.94
2	B	104	HEC	C3B-C4B-NB	6.86	123.90	110.94
2	A	104	HEC	CAA-C2A-C3A	4.73	140.83	127.25
2	B	104	HEC	CAA-C2A-C3A	4.73	140.83	127.25
2	A	104	HEC	CAD-C3D-C2D	-4.13	115.37	127.25
2	B	104	HEC	CAD-C3D-C2D	-4.13	115.37	127.25
2	A	104	HEC	CBA-CAA-C2A	3.81	119.50	112.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	104	HEC	CBA-CAA-C2A	3.81	119.50	112.48
2	A	104	HEC	CMB-C2B-C3B	3.36	129.77	125.82
2	B	104	HEC	CMB-C2B-C3B	3.36	129.77	125.82
2	A	104	HEC	CMA-C3A-C2A	2.27	129.23	124.94
2	B	104	HEC	CMA-C3A-C2A	2.27	129.23	124.94

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	104	HEC	C1A-C2A-CAA-CBA
2	A	104	HEC	C3A-C2A-CAA-CBA
2	A	104	HEC	C2D-C3D-CAD-CBD
2	A	104	HEC	C4D-C3D-CAD-CBD
2	B	104	HEC	C1A-C2A-CAA-CBA
2	B	104	HEC	C3A-C2A-CAA-CBA
2	B	104	HEC	C2D-C3D-CAD-CBD
2	B	104	HEC	C4D-C3D-CAD-CBD

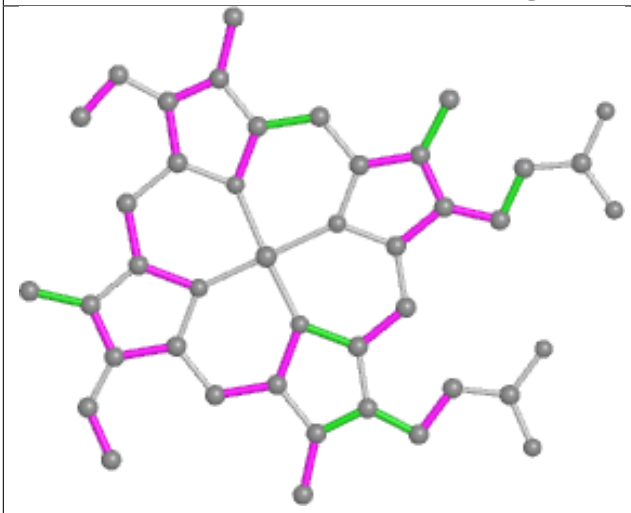
There are no ring outliers.

2 monomers are involved in 46 short contacts:

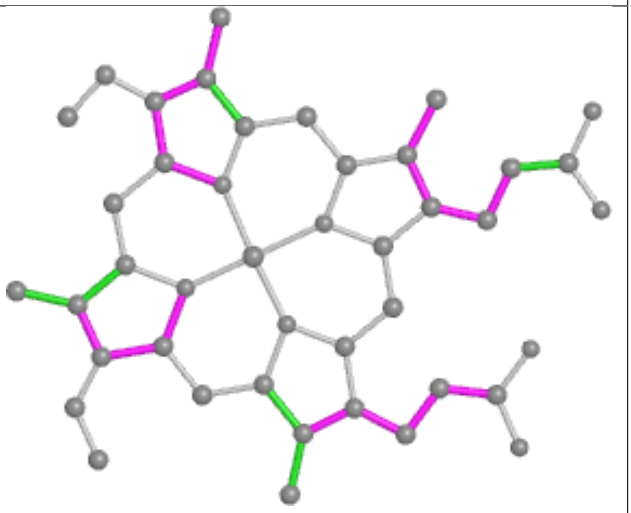
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	104	HEC	23	0
2	A	104	HEC	23	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

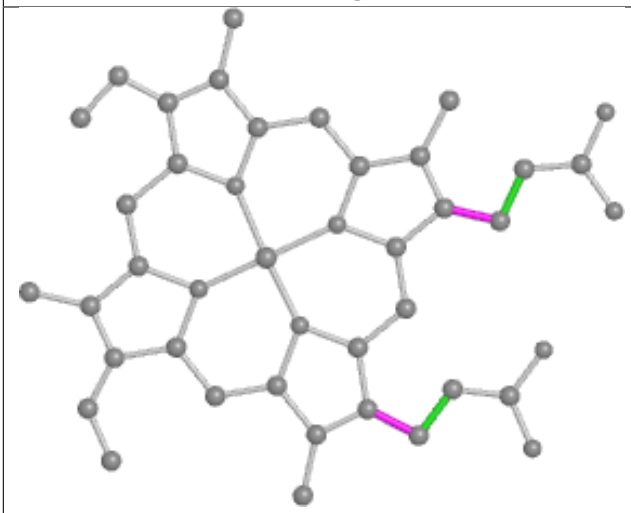
Ligand HEC B 104



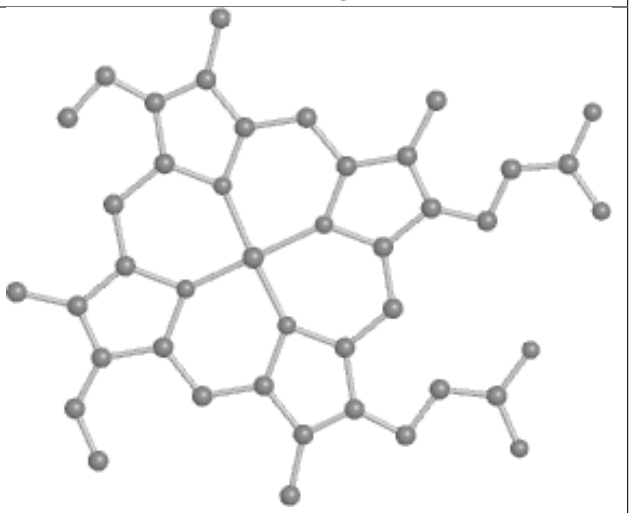
Bond lengths



Bond angles

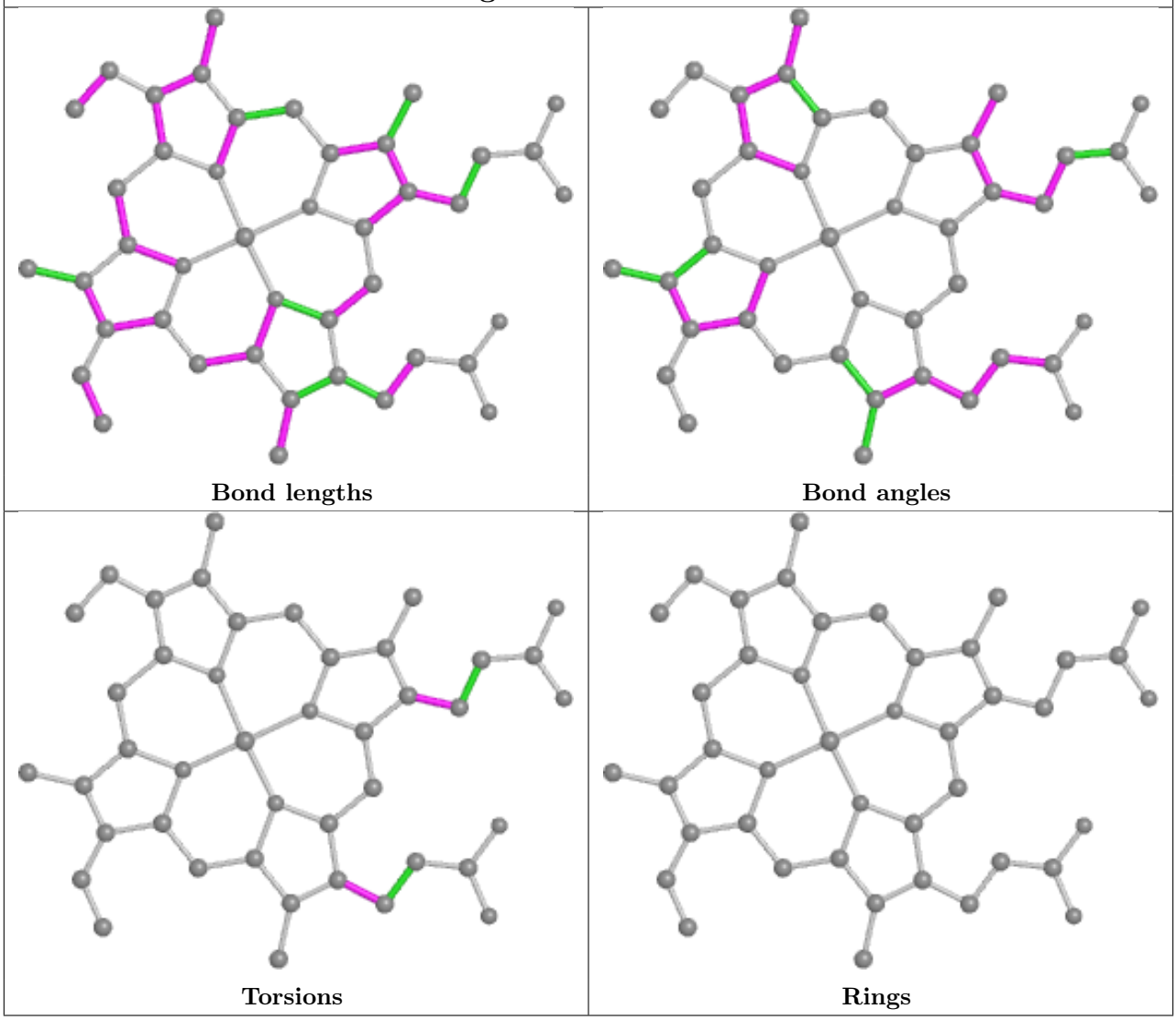


Torsions



Rings

Ligand HEC A 104



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	29
1	B	29

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	26:HIS	C	27:LYS	N	1.20
1	A	31:ASN	C	32:LEU	N	1.20
1	A	50:ASP	C	51:ALA	N	1.20
1	A	80:MET	C	81:ILE	N	1.20
1	B	26:HIS	C	27:LYS	N	1.20
1	B	31:ASN	C	32:LEU	N	1.20
1	B	50:ASP	C	51:ALA	N	1.20
1	B	80:MET	C	81:ILE	N	1.20
1	A	61:GLU	C	62:ASN	N	1.19
1	A	101:ALA	C	102:THR	N	1.19
1	A	102:THR	C	103:SER	N	1.19
1	B	61:GLU	C	62:ASN	N	1.19
1	B	101:ALA	C	102:THR	N	1.19
1	B	102:THR	C	103:SER	N	1.19
1	A	8:LYS	C	9:THR	N	1.18
1	A	35:LEU	C	36:PHE	N	1.18
1	A	78:THR	C	79:LYS	N	1.18
1	A	97:TYR	C	98:LEU	N	1.18
1	B	8:LYS	C	9:THR	N	1.18
1	B	35:LEU	C	36:PHE	N	1.18
1	B	78:THR	C	79:LYS	N	1.18
1	B	97:TYR	C	98:LEU	N	1.18
1	A	19:THR	C	20:VAL	N	1.17
1	A	54:SER	C	55:LYS	N	1.17
1	B	19:THR	C	20:VAL	N	1.17
1	B	54:SER	C	55:LYS	N	1.17
1	A	12:GLN	C	13:LYS	N	1.16
1	A	55:LYS	C	56:GLY	N	1.16
1	B	12:GLN	C	13:LYS	N	1.16
1	B	55:LYS	C	56:GLY	N	1.16
1	A	60:ASN	C	61:GLU	N	1.15
1	A	90:GLU	C	91:ARG	N	1.15
1	B	60:ASN	C	61:GLU	N	1.15
1	B	90:GLU	C	91:ARG	N	1.15
1	A	65:MET	C	66:GLU	N	1.14
1	A	69:GLU	C	70:ASN	N	1.14
1	B	65:MET	C	66:GLU	N	1.14
1	B	69:GLU	C	70:ASN	N	1.14
1	A	46:TYR	C	47:SER	N	1.13
1	A	66:GLU	C	67:TYR	N	1.13
1	A	82:PHE	C	83:ALA	N	1.13
1	A	89:GLY	C	90:GLU	N	1.13
1	B	46:TYR	C	47:SER	N	1.13

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	66:GLU	C	67:TYR	N	1.13
1	B	82:PHE	C	83:ALA	N	1.13
1	B	89:GLY	C	90:GLU	N	1.13
1	A	22:ASN	C	23:GLY	N	1.11
1	B	22:ASN	C	23:GLY	N	1.11
1	A	86:LYS	C	87:LYS	N	1.09
1	B	86:LYS	C	87:LYS	N	1.09
1	A	40:THR	C	41:GLY	N	1.08
1	A	59:TRP	C	60:ASN	N	1.08
1	A	93:ASP	C	94:LEU	N	1.08
1	B	40:THR	C	41:GLY	N	1.08
1	B	59:TRP	C	60:ASN	N	1.08
1	B	93:ASP	C	94:LEU	N	1.08
1	A	32:LEU	C	33:TRP	N	1.05
1	B	32:LEU	C	33:TRP	N	1.05

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.