



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 10:03 AM EDT

PDB ID : 1FOC / pdb_00001foc
Title : Cytochrome C557: improperly folded thermus thermophilus C552
Authors : McRee, D.E.; Williams, P.A.; Fee, J.A.; Bren, K.L.
Deposited on : 2000-08-27
Resolution : 3.00 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

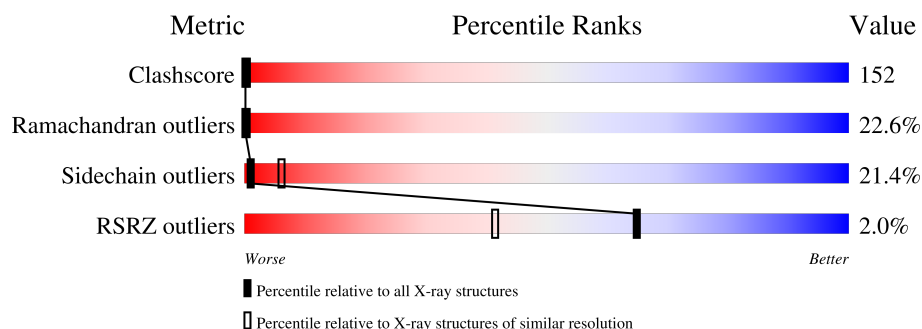
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	132	2% 5% 33% 47% 13% .
1	B	132	2% . 38% 45% 11% .

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:

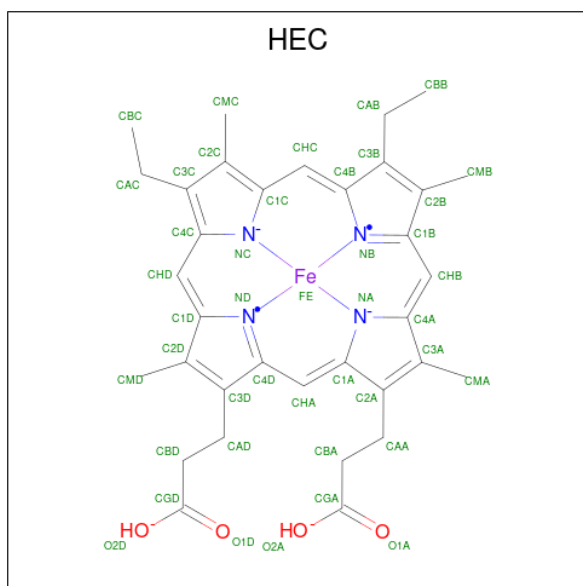
Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	HEC	A	200	X	-	-	-
2	HEC	B	200	X	-	-	-

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 CYTOCHROME RC557.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	128	Total 972	C 626	N 171	O 171	S 4	29	0	0
1	B	128	Total 972	C 626	N 171	O 171	S 4	29	0	0

- Molecule 2 is HEME C (CCD ID: HEC) (formula: $\text{C}_{34}\text{H}_{36}\text{FeN}_4\text{O}_4$).

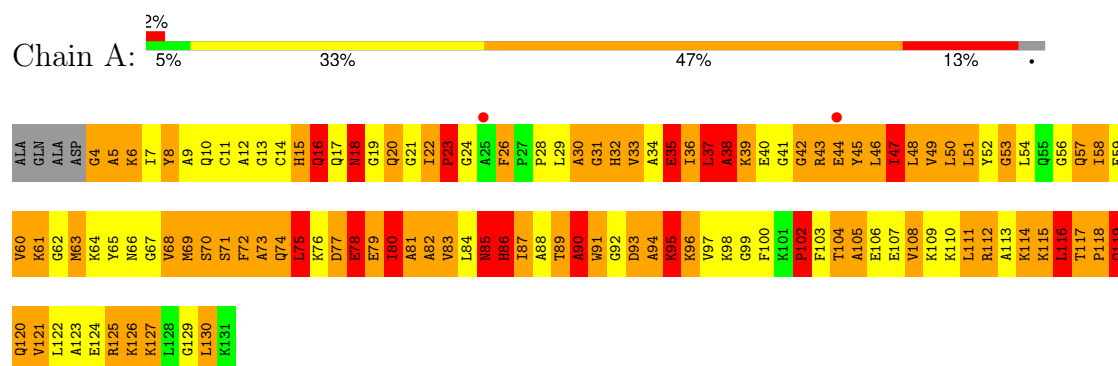


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

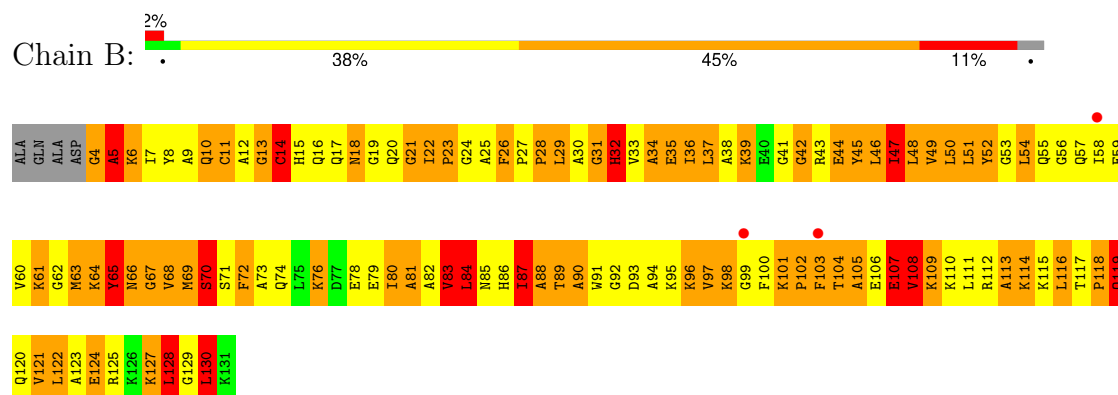
3 Residue-property plots

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

• Molecule 1: CYTOCHROME RC557



• Molecule 1: CYTOCHROME RC557



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	98.72Å 69.05Å 36.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.00 40.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.00) 98.1 (40.00-3.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 3.01Å)	Xtriage
Refinement program	XTALVIEW, CNS 0.9	Depositor
R, R_{free}	0.273 , 0.423 0.279 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	102.2	Xtriage
Anisotropy	0.187	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 163.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	2030	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.77% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.95	20/989 (2.0%)	2.21	43/1325 (3.2%)
1	B	1.94	22/989 (2.2%)	2.33	51/1325 (3.8%)
All	All	1.94	42/1978 (2.1%)	2.27	94/2650 (3.5%)

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	B	0	1

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	44	GLU	C-N	17.00	1.55	1.33
1	A	63	MET	SD-CE	16.82	2.21	1.79
1	B	69	MET	SD-CE	-14.68	1.42	1.79
1	A	108	VAL	CA-CB	-9.64	1.42	1.54
1	A	69	MET	CA-C	-9.52	1.40	1.52
1	A	49	VAL	CA-CB	-9.01	1.42	1.54
1	A	121	VAL	CA-CB	-8.99	1.41	1.54
1	B	83	VAL	CA-C	-8.30	1.42	1.52
1	B	88	ALA	CA-CB	8.05	1.67	1.53
1	B	54	LEU	CA-C	7.68	1.61	1.52
1	A	47	ILE	CA-CB	7.63	1.64	1.54
1	B	49	VAL	CA-CB	-7.53	1.46	1.54
1	B	69	MET	C-O	-7.38	1.15	1.23
1	A	60	VAL	CA-CB	-7.25	1.44	1.54
1	B	81	ALA	C-O	7.19	1.33	1.24
1	A	108	VAL	N-CA	-6.97	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	89	THR	CA-C	6.86	1.59	1.52
1	B	90	ALA	CA-CB	-6.39	1.42	1.53
1	A	121	VAL	CB-CG1	-6.37	1.31	1.52
1	B	103	PHE	N-CA	-6.33	1.39	1.46
1	B	4	GLY	N-CA	6.10	1.55	1.45
1	A	15	HIS	CA-CB	6.04	1.62	1.53
1	B	68	VAL	CA-CB	-5.99	1.45	1.55
1	A	46	LEU	CA-C	5.92	1.60	1.52
1	B	46	LEU	CA-C	-5.92	1.45	1.52
1	B	66	ASN	CB-CG	5.91	1.66	1.52
1	B	69	MET	CG-SD	-5.79	1.66	1.80
1	B	128	LEU	CA-C	5.77	1.60	1.52
1	B	121	VAL	CA-CB	-5.71	1.45	1.54
1	A	4	GLY	N-CA	5.64	1.54	1.45
1	B	14	CYS	C-O	-5.46	1.17	1.24
1	A	74	GLN	CA-C	-5.45	1.46	1.52
1	B	69	MET	CA-C	-5.44	1.46	1.53
1	B	72	PHE	CA-C	-5.39	1.45	1.53
1	B	84	LEU	CA-C	5.32	1.60	1.52
1	B	89	THR	CA-CB	-5.24	1.45	1.53
1	A	71	SER	CA-C	-5.23	1.46	1.52
1	A	82	ALA	CA-CB	-5.12	1.47	1.53
1	A	86	HIS	C-N	-5.08	1.28	1.34
1	A	43	ARG	C-N	5.05	1.40	1.33
1	A	121	VAL	CA-C	-5.01	1.45	1.52
1	B	15	HIS	CA-CB	-5.00	1.45	1.53

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	43	ARG	CA-C-N	15.74	141.85	120.44
1	A	43	ARG	C-N-CA	15.74	141.85	120.44
1	B	18	ASN	N-CA-C	-15.52	94.42	113.20
1	B	83	VAL	N-CA-C	-14.93	96.09	110.42
1	A	20	GLN	N-CA-C	-12.71	97.08	111.82
1	B	6	LYS	N-CA-C	-12.29	96.41	111.40
1	B	53	GLY	CA-C-O	-11.85	113.72	122.37
1	B	122	LEU	N-CA-C	-11.10	98.95	111.71
1	A	6	LYS	N-CA-C	-11.01	99.25	111.14
1	B	130	LEU	N-CA-C	10.88	125.94	109.41
1	B	46	LEU	N-CA-C	-10.80	98.15	111.11
1	A	29	LEU	N-CA-C	-10.66	98.80	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	53	GLY	N-CA-C	-10.55	101.93	111.95
1	A	85	ASN	N-CA-C	-10.19	100.64	112.87
1	A	72	PHE	N-CA-C	-10.01	99.36	112.68
1	A	105	ALA	N-CA-C	9.38	122.50	111.71
1	A	24	GLY	N-CA-C	-9.32	103.61	113.58
1	A	121	VAL	CA-C-N	-9.30	107.08	120.29
1	A	121	VAL	C-N-CA	-9.30	107.08	120.29
1	B	29	LEU	N-CA-C	-9.21	102.17	113.41
1	B	53	GLY	N-CA-C	-9.08	102.91	112.08
1	B	81	ALA	CA-C-O	9.03	129.00	118.79
1	A	18	ASN	N-CA-C	8.92	123.95	112.89
1	B	68	VAL	CB-CA-C	-8.66	95.67	110.30
1	B	13	GLY	N-CA-C	-8.50	97.43	112.22
1	B	98	LYS	N-CA-C	8.50	123.06	110.48
1	B	97	VAL	N-CA-C	8.34	119.89	108.89
1	B	66	ASN	N-CA-C	-8.28	101.19	113.61
1	B	26	PHE	CA-C-N	-8.07	112.06	120.38
1	B	26	PHE	C-N-CA	-8.07	112.06	120.38
1	A	117	THR	N-CA-C	8.02	122.38	108.82
1	B	81	ALA	N-CA-C	-7.95	101.76	114.09
1	B	11	CYS	N-CA-C	7.77	125.27	107.48
1	B	21	GLY	N-CA-C	-7.73	98.14	112.37
1	A	117	THR	CA-C-N	7.62	129.37	119.84
1	A	117	THR	C-N-CA	7.62	129.37	119.84
1	A	44	GLU	O-C-N	7.56	130.26	122.09
1	B	52	TYR	N-CA-C	7.55	122.78	113.50
1	A	69	MET	N-CA-C	-7.49	95.94	108.75
1	B	87	ILE	N-CA-C	-7.30	101.92	111.05
1	A	119	GLN	N-CA-C	-7.25	104.42	113.55
1	B	44	GLU	N-CA-C	-7.07	95.75	110.80
1	A	120	GLN	N-CA-C	-7.05	99.73	111.37
1	A	47	ILE	CB-CA-C	-6.95	99.89	111.29
1	B	109	LYS	N-CA-C	-6.95	102.85	111.75
1	B	22	ILE	N-CA-C	6.86	123.69	108.88
1	A	32	HIS	N-CA-C	-6.79	103.11	111.33
1	B	32	HIS	N-CA-C	6.78	125.23	110.80
1	B	34	ALA	N-CA-C	-6.69	103.99	111.28
1	A	32	HIS	CA-C-N	-6.63	109.74	120.62
1	A	32	HIS	C-N-CA	-6.63	109.74	120.62
1	B	76	LYS	CA-C-N	6.61	129.42	120.44
1	B	76	LYS	C-N-CA	6.61	129.42	120.44
1	B	48	LEU	O-C-N	6.60	129.67	122.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	36	ILE	N-CA-C	-6.27	104.17	113.39
1	B	49	VAL	CB-CA-C	-6.26	103.68	111.70
1	A	74	GLN	N-CA-C	-6.25	104.72	112.72
1	B	108	VAL	CB-CA-C	-6.18	101.15	111.29
1	B	64	LYS	N-CA-C	-6.15	99.37	109.40
1	A	78	GLU	N-CA-C	-6.15	97.71	110.80
1	B	27	PRO	CA-C-N	6.14	128.54	120.25
1	B	27	PRO	C-N-CA	6.14	128.54	120.25
1	B	103	PHE	CB-CA-C	6.05	121.42	111.50
1	A	16	GLN	N-CA-C	6.03	123.64	110.80
1	B	101	LYS	N-CA-C	6.01	119.76	109.06
1	B	5	ALA	N-CA-C	-5.99	98.04	110.80
1	B	65	TYR	N-CA-C	-5.98	101.35	110.14
1	A	26	PHE	CA-C-N	-5.93	114.27	120.38
1	A	26	PHE	C-N-CA	-5.93	114.27	120.38
1	A	116	LEU	N-CA-C	5.80	119.05	109.94
1	B	51	LEU	N-CA-C	5.74	117.34	111.14
1	A	75	LEU	N-CA-C	-5.65	102.17	110.42
1	B	119	GLN	N-CA-C	-5.57	105.11	111.07
1	A	112	ARG	N-CA-C	-5.55	105.33	111.71
1	B	37	LEU	CA-CB-CG	-5.50	97.04	116.30
1	B	47	ILE	CB-CA-C	-5.50	103.64	112.16
1	B	48	LEU	CA-C-N	5.47	127.94	120.77
1	B	48	LEU	C-N-CA	5.47	127.94	120.77
1	B	107	GLU	CA-C-N	5.47	131.82	121.97
1	B	107	GLU	C-N-CA	5.47	131.82	121.97
1	B	61	LYS	N-CA-C	-5.47	105.69	112.47
1	A	37	LEU	CA-CB-CG	-5.41	97.38	116.30
1	A	95	LYS	N-CA-C	-5.39	99.31	110.80
1	A	61	LYS	N-CA-C	-5.32	103.67	111.17
1	B	35	GLU	N-CA-C	5.31	116.87	111.14
1	B	74	GLN	N-CA-C	5.15	121.77	110.80
1	A	45	TYR	CA-C-O	5.14	126.22	120.82
1	A	38	ALA	N-CA-C	-5.13	99.88	110.80
1	A	86	HIS	CA-C-N	-5.06	114.24	121.52
1	A	86	HIS	C-N-CA	-5.06	114.24	121.52
1	A	12	ALA	CA-C-N	-5.02	117.45	122.63
1	A	12	ALA	C-N-CA	-5.02	117.45	122.63
1	A	90	ALA	N-CA-C	5.01	121.48	110.80
1	B	31	GLY	N-CA-C	-5.01	101.31	113.18

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	65	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	972	0	1015	289	0
1	B	972	0	1015	320	0
2	A	43	0	31	7	0
2	B	43	0	31	14	0
All	All	2030	0	2092	606	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 152.

All (606) 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:63:MET:SD	1:A:63:MET:CE	2.21	1.27
1:B:36:ILE:O	1:B:42:GLY:HA3	1.35	1.25
1:A:15:HIS:C	1:A:21:GLY:HA2	1.68	1.18
1:B:57:GLN:HA	1:B:65:TYR:O	1.42	1.17
1:B:37:LEU:HD23	1:B:43:ARG:HG2	1.26	1.14
1:B:45:TYR:HA	1:B:48:LEU:HD12	1.31	1.13
1:B:55:GLN:CG	1:B:118:PRO:HB3	1.79	1.11
1:B:48:LEU:HD23	1:B:52:TYR:HE2	1.16	1.10
1:A:95:LYS:HG3	1:A:96:LYS:H	0.94	1.10
1:A:80:ILE:O	1:A:82:ALA:N	1.85	1.09
1:B:4:GLY:HA2	1:B:82:ALA:HB1	1.36	1.07
1:B:6:LYS:O	1:B:9:ALA:HB3	1.54	1.07
1:A:16:GLN:HA	1:A:16:GLN:HE21	1.17	1.05
1:A:75:LEU:HA	1:A:79:GLU:OE1	1.56	1.04
1:A:32:HIS:HA	1:A:35:GLU:OE2	1.56	1.03
1:B:23:PRO:O	1:B:25:ALA:N	1.90	1.03
1:A:44:GLU:O	1:A:48:LEU:HG	1.56	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:LYS:CG	1:A:96:LYS:H	1.66	1.02
1:A:16:GLN:HE21	1:A:16:GLN:CA	1.73	1.01
1:B:47:ILE:HG22	1:B:51:LEU:HD12	1.39	1.01
1:B:34:ALA:HB3	1:B:35:GLU:OE1	1.58	1.00
1:B:55:GLN:HG3	1:B:118:PRO:CB	1.91	1.00
1:B:48:LEU:HD23	1:B:52:TYR:CE2	1.95	1.00
1:A:75:LEU:HB3	1:A:79:GLU:HB3	1.43	0.99
1:B:36:ILE:H	1:B:36:ILE:HD12	1.28	0.98
1:B:104:THR:O	1:B:106:GLU:N	1.96	0.97
1:B:60:VAL:O	1:B:60:VAL:HG13	1.64	0.97
1:A:32:HIS:NE2	1:A:36:ILE:HD11	1.79	0.96
1:A:45:TYR:CE2	1:A:125:ARG:HB2	1.99	0.96
1:B:85:ASN:O	1:B:89:THR:HG23	1.65	0.95
1:B:45:TYR:O	1:B:48:LEU:N	1.99	0.95
1:B:82:ALA:O	1:B:85:ASN:N	2.00	0.94
1:B:95:LYS:O	1:B:96:LYS:HG3	1.66	0.94
1:A:34:ALA:O	1:A:37:LEU:N	2.00	0.94
1:A:77:ASP:HA	1:A:108:VAL:HG11	1.48	0.94
1:B:83:VAL:HG21	2:B:200:HEC:HBC2	1.49	0.94
1:B:117:THR:OG1	1:B:120:GLN:HG3	1.68	0.94
1:A:95:LYS:HG3	1:A:96:LYS:N	1.80	0.93
1:A:89:THR:HG22	1:A:94:ALA:HB2	1.51	0.93
1:A:80:ILE:HG22	1:A:81:ALA:H	1.32	0.93
1:B:76:LYS:N	1:B:76:LYS:HD2	1.84	0.93
1:A:6:LYS:O	1:A:9:ALA:HB3	1.68	0.93
1:B:85:ASN:O	1:B:88:ALA:HB3	1.67	0.93
1:B:108:VAL:HG12	1:B:109:LYS:N	1.84	0.93
1:B:83:VAL:HG22	1:B:84:LEU:N	1.86	0.91
1:B:55:GLN:HG3	1:B:118:PRO:HB3	0.94	0.90
1:B:85:ASN:C	1:B:88:ALA:HB3	1.96	0.90
1:B:20:GLN:HG2	1:B:21:GLY:O	1.72	0.90
1:B:104:THR:C	1:B:106:GLU:H	1.79	0.90
1:A:80:ILE:HG22	1:A:81:ALA:N	1.85	0.88
1:A:16:GLN:HG2	1:A:21:GLY:O	1.73	0.88
1:B:120:GLN:O	1:B:123:ALA:HB3	1.72	0.88
1:A:45:TYR:CZ	1:A:125:ARG:HB2	2.07	0.87
1:B:76:LYS:HD2	1:B:76:LYS:H	1.38	0.87
1:A:82:ALA:C	1:A:84:LEU:H	1.81	0.87
1:A:86:HIS:C	1:A:86:HIS:CD2	2.53	0.86
1:B:113:ALA:O	1:B:115:LYS:N	2.09	0.86
1:B:113:ALA:O	1:B:115:LYS:HG3	1.76	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:HIS:CD2	1:A:36:ILE:HD11	2.09	0.86
1:B:42:GLY:O	1:B:46:LEU:HG	1.76	0.85
1:A:124:GLU:HA	1:A:127:LYS:HG3	1.57	0.85
1:A:10:GLN:O	1:B:10:GLN:CB	2.25	0.84
1:B:37:LEU:CD2	1:B:43:ARG:HG2	2.07	0.84
1:A:85:ASN:HD21	1:A:103:PHE:H	1.23	0.84
1:B:36:ILE:O	1:B:42:GLY:CA	2.24	0.83
1:B:41:GLY:O	1:B:43:ARG:N	2.11	0.83
1:A:6:LYS:H	1:A:6:LYS:HD2	1.44	0.83
1:A:111:LEU:HD23	1:A:114:LYS:HG3	1.60	0.83
1:B:47:ILE:CG2	1:B:51:LEU:HD12	2.07	0.83
1:A:75:LEU:HD12	1:A:80:ILE:HG13	1.58	0.83
1:A:93:ASP:C	1:A:95:LYS:H	1.85	0.83
1:B:44:GLU:O	1:B:47:ILE:N	2.12	0.83
1:A:82:ALA:O	1:A:84:LEU:N	2.12	0.82
1:A:16:GLN:OE1	1:A:22:ILE:HB	1.80	0.82
1:B:32:HIS:H	1:B:61:LYS:HZ1	1.25	0.82
1:A:45:TYR:O	1:A:48:LEU:HB2	1.80	0.81
1:B:79:GLU:O	1:B:82:ALA:HB3	1.81	0.81
1:A:117:THR:O	1:A:120:GLN:N	2.12	0.81
1:B:44:GLU:HB3	1:B:111:LEU:HD22	1.60	0.81
1:A:75:LEU:HB3	1:A:79:GLU:CB	2.10	0.81
1:B:58:ILE:O	1:B:64:LYS:HA	1.80	0.80
1:A:117:THR:OG1	1:A:120:GLN:HG3	1.82	0.80
1:B:108:VAL:CG1	1:B:112:ARG:HD2	2.11	0.80
1:A:15:HIS:O	1:A:21:GLY:HA2	1.81	0.80
1:A:114:LYS:O	1:A:116:LEU:HD23	1.81	0.80
1:A:16:GLN:OE1	1:A:22:ILE:HD12	1.82	0.80
1:A:93:ASP:O	1:A:95:LYS:N	2.14	0.80
1:B:36:ILE:HD12	1:B:36:ILE:N	1.96	0.80
1:B:22:ILE:O	1:B:23:PRO:O	2.01	0.79
1:A:20:GLN:O	1:A:23:PRO:HD3	1.83	0.79
1:B:51:LEU:HD21	1:B:112:ARG:NH2	1.97	0.79
1:A:75:LEU:HB2	1:A:80:ILE:HD12	1.65	0.78
1:A:77:ASP:HA	1:A:108:VAL:CG1	2.13	0.78
1:A:32:HIS:HE2	1:A:36:ILE:HD11	1.46	0.78
1:B:16:GLN:C	1:B:17:GLN:HE21	1.92	0.78
1:B:116:LEU:O	1:B:117:THR:HG23	1.83	0.78
1:A:16:GLN:CA	1:A:16:GLN:NE2	2.42	0.77
1:A:85:ASN:ND2	1:A:103:PHE:H	1.81	0.77
1:B:106:GLU:C	1:B:108:VAL:H	1.91	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:ALA:O	1:A:91:TRP:CD1	2.36	0.77
1:A:7:ILE:HG22	1:A:83:VAL:HG21	1.65	0.77
1:A:77:ASP:OD2	1:A:109:LYS:HB2	1.85	0.77
1:A:77:ASP:OD1	1:A:108:VAL:HG12	1.85	0.77
1:A:93:ASP:C	1:A:95:LYS:N	2.41	0.77
1:B:100:PHE:C	1:B:101:LYS:HD2	2.09	0.77
1:A:117:THR:O	1:A:119:GLN:N	2.18	0.76
1:A:4:GLY:N	1:A:6:LYS:HD3	2.00	0.76
1:B:36:ILE:H	1:B:36:ILE:CD1	1.98	0.76
1:A:52:TYR:CD2	1:A:116:LEU:HB2	2.21	0.76
1:B:127:LYS:O	1:B:129:GLY:N	2.19	0.76
1:B:44:GLU:HG3	1:B:111:LEU:HD11	1.66	0.76
1:B:41:GLY:HA2	1:B:44:GLU:OE1	1.85	0.76
1:A:98:LYS:O	1:A:100:PHE:N	2.19	0.75
1:B:60:VAL:O	1:B:60:VAL:CG1	2.33	0.75
1:B:28:PRO:HD2	1:B:60:VAL:HG21	1.69	0.75
1:B:76:LYS:H	1:B:76:LYS:CD	1.97	0.75
1:B:6:LYS:H	1:B:6:LYS:HD2	1.52	0.75
1:B:41:GLY:O	1:B:44:GLU:N	2.20	0.75
1:A:120:GLN:O	1:A:123:ALA:HB3	1.86	0.74
1:B:44:GLU:HG2	1:B:111:LEU:HD21	1.68	0.74
1:B:100:PHE:O	1:B:101:LYS:HD2	1.87	0.74
1:A:78:GLU:O	1:A:80:ILE:N	2.20	0.74
1:B:47:ILE:O	1:B:51:LEU:HB2	1.87	0.74
1:B:4:GLY:CA	1:B:82:ALA:HB1	2.14	0.74
1:B:32:HIS:N	1:B:61:LYS:NZ	2.35	0.74
1:B:80:ILE:O	1:B:80:ILE:HG22	1.87	0.74
1:B:45:TYR:C	1:B:48:LEU:H	1.96	0.73
1:B:45:TYR:CA	1:B:48:LEU:HD12	2.15	0.73
1:A:16:GLN:CG	1:A:21:GLY:O	2.36	0.73
1:B:23:PRO:C	1:B:25:ALA:H	1.95	0.73
1:B:28:PRO:CD	1:B:60:VAL:HG21	2.19	0.73
1:A:51:LEU:O	1:A:73:ALA:HB2	1.89	0.72
1:B:101:LYS:HB3	1:B:102:PRO:HD2	1.71	0.72
1:B:56:GLY:HA3	1:B:122:LEU:HD22	1.69	0.72
1:B:84:LEU:O	1:B:88:ALA:HB2	1.88	0.72
1:A:16:GLN:HE21	1:A:16:GLN:N	1.88	0.72
1:A:20:GLN:O	1:A:23:PRO:CD	2.38	0.72
1:B:106:GLU:O	1:B:108:VAL:N	2.23	0.72
1:B:114:LYS:HB3	1:B:116:LEU:CD2	2.20	0.72
1:A:86:HIS:CD2	1:A:86:HIS:O	2.42	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:HIS:N	1:B:61:LYS:HZ1	1.88	0.71
1:A:107:GLU:O	1:A:111:LEU:HD12	1.90	0.71
1:B:22:ILE:O	1:B:22:ILE:HG13	1.88	0.71
1:A:16:GLN:HB2	1:A:21:GLY:CA	2.21	0.71
1:B:108:VAL:CG1	1:B:109:LYS:N	2.52	0.71
1:B:41:GLY:O	1:B:42:GLY:C	2.34	0.71
1:A:16:GLN:NE2	1:A:16:GLN:N	2.38	0.71
1:A:18:ASN:ND2	1:A:20:GLN:HB3	2.05	0.71
1:A:86:HIS:O	1:A:86:HIS:HD2	1.74	0.71
1:B:9:ALA:O	1:B:11:CYS:N	2.24	0.70
1:A:43:ARG:O	1:A:47:ILE:HG12	1.92	0.70
1:A:41:GLY:O	1:A:44:GLU:N	2.23	0.70
1:A:116:LEU:HD13	1:A:120:GLN:HB3	1.74	0.70
1:A:16:GLN:HB2	1:A:21:GLY:HA2	1.73	0.70
1:A:95:LYS:O	1:A:97:VAL:O	2.09	0.70
1:B:22:ILE:HD12	1:B:23:PRO:CD	2.20	0.70
1:B:108:VAL:HG13	1:B:112:ARG:HD2	1.74	0.69
1:B:83:VAL:HG21	2:B:200:HEC:CBC	2.21	0.69
1:A:117:THR:OG1	1:A:120:GLN:CG	2.40	0.69
1:A:57:GLN:HA	1:A:66:ASN:HA	1.75	0.69
1:A:69:MET:HB2	2:A:200:HEC:C4A	2.23	0.69
1:B:93:ASP:HA	1:B:96:LYS:CE	2.23	0.68
1:A:58:ILE:HB	1:A:125:ARG:NH1	2.08	0.68
1:A:17:GLN:O	1:A:17:GLN:HG2	1.94	0.68
1:B:36:ILE:HG21	1:B:46:LEU:HD21	1.75	0.68
1:A:4:GLY:N	1:A:6:LYS:HZ3	1.92	0.68
1:A:7:ILE:CG2	1:A:83:VAL:HG21	2.24	0.68
1:B:76:LYS:O	1:B:80:ILE:HG13	1.94	0.68
1:A:16:GLN:NE2	1:A:16:GLN:H	1.91	0.68
1:B:69:MET:HE1	2:B:200:HEC:NC	2.07	0.68
1:A:82:ALA:C	1:A:84:LEU:N	2.52	0.68
1:B:39:LYS:HE3	1:B:130:LEU:HD21	1.75	0.68
1:A:95:LYS:O	1:A:97:VAL:N	2.27	0.67
1:B:106:GLU:C	1:B:108:VAL:N	2.49	0.67
1:A:84:LEU:C	1:A:86:HIS:N	2.50	0.67
1:B:20:GLN:O	1:B:28:PRO:HB3	1.95	0.67
1:B:94:ALA:HB2	1:B:100:PHE:CZ	2.29	0.67
1:B:113:ALA:O	1:B:114:LYS:C	2.38	0.67
1:B:22:ILE:HD12	1:B:23:PRO:HD2	1.74	0.67
1:B:119:GLN:O	1:B:122:LEU:HB3	1.93	0.67
1:B:123:ALA:O	1:B:125:ARG:N	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:LYS:HB3	1:B:116:LEU:HD21	1.75	0.67
1:B:50:LEU:HD21	2:B:200:HEC:HBC3	1.76	0.67
1:A:51:LEU:O	1:A:71:SER:OG	2.11	0.66
1:A:6:LYS:H	1:A:6:LYS:CD	2.08	0.66
1:B:4:GLY:N	1:B:6:LYS:HD3	2.09	0.66
1:A:51:LEU:HD21	1:A:112:ARG:HD3	1.78	0.66
1:B:108:VAL:O	1:B:112:ARG:HG3	1.95	0.66
1:B:120:GLN:O	1:B:123:ALA:CB	2.43	0.66
1:A:51:LEU:C	1:A:71:SER:OG	2.39	0.66
1:B:6:LYS:O	1:B:9:ALA:CB	2.38	0.66
1:A:75:LEU:HD12	1:A:80:ILE:CG1	2.26	0.65
1:B:11:CYS:O	1:B:13:GLY:O	2.13	0.65
1:B:20:GLN:O	1:B:28:PRO:CA	2.43	0.65
1:B:17:GLN:C	1:B:19:GLY:H	2.04	0.65
1:B:127:LYS:O	1:B:128:LEU:C	2.38	0.65
1:B:48:LEU:CD2	1:B:52:TYR:HE2	2.04	0.65
1:A:112:ARG:O	1:A:115:LYS:HG3	1.96	0.65
1:B:16:GLN:CG	1:B:21:GLY:H	2.09	0.65
1:B:83:VAL:CG2	2:B:200:HEC:HBC2	2.25	0.65
1:A:16:GLN:HA	1:A:16:GLN:NE2	1.98	0.64
1:B:80:ILE:O	1:B:84:LEU:HD12	1.97	0.64
1:A:122:LEU:O	1:A:125:ARG:N	2.24	0.64
1:A:86:HIS:C	1:A:86:HIS:HD2	2.00	0.64
1:B:102:PRO:O	1:B:104:THR:N	2.30	0.64
1:A:5:ALA:HA	1:A:86:HIS:ND1	2.12	0.64
1:A:54:LEU:HD11	1:A:122:LEU:HD13	1.79	0.63
1:B:17:GLN:C	1:B:19:GLY:N	2.53	0.63
1:B:81:ALA:HB1	1:B:103:PHE:O	1.97	0.63
1:B:45:TYR:O	1:B:49:VAL:HG23	1.97	0.63
1:B:72:PHE:HZ	2:B:200:HEC:HBB3	1.63	0.63
1:B:116:LEU:HD12	1:B:121:VAL:HG22	1.81	0.63
1:B:41:GLY:C	1:B:43:ARG:N	2.54	0.63
1:B:95:LYS:O	1:B:95:LYS:HG3	1.97	0.63
1:A:51:LEU:HA	1:A:73:ALA:HB2	1.81	0.63
1:A:117:THR:N	1:A:120:GLN:HG3	2.13	0.63
1:B:9:ALA:C	1:B:11:CYS:H	2.07	0.63
1:B:28:PRO:HD2	1:B:60:VAL:CG2	2.29	0.63
1:A:36:ILE:O	1:A:42:GLY:HA3	1.99	0.63
1:B:7:ILE:HG21	1:B:83:VAL:HG12	1.80	0.63
1:B:80:ILE:O	1:B:80:ILE:CG2	2.47	0.62
1:B:92:GLY:O	1:B:96:LYS:HE2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:GLU:OE1	1:B:35:GLU:N	2.32	0.62
1:A:16:GLN:OE1	1:A:22:ILE:CG1	2.47	0.62
1:A:16:GLN:OE1	1:A:22:ILE:CB	2.47	0.62
1:A:77:ASP:O	1:A:78:GLU:O	2.17	0.62
1:B:35:GLU:OE2	1:B:61:LYS:HD3	1.98	0.62
1:B:97:VAL:HB	1:B:100:PHE:HD1	1.65	0.62
1:A:19:GLY:HA2	1:A:91:TRP:CH2	2.35	0.62
1:B:113:ALA:C	1:B:115:LYS:N	2.57	0.62
1:B:7:ILE:HD12	1:B:82:ALA:HB3	1.82	0.62
1:A:22:ILE:HG22	1:A:26:PHE:HD1	1.65	0.61
1:A:16:GLN:OE1	1:A:22:ILE:CD1	2.48	0.61
1:A:75:LEU:CD1	1:A:80:ILE:HG13	2.28	0.61
1:B:20:GLN:O	1:B:28:PRO:HA	2.00	0.61
1:B:108:VAL:C	1:B:110:LYS:N	2.54	0.61
1:A:45:TYR:HA	1:A:48:LEU:HD12	1.81	0.61
1:B:57:GLN:CA	1:B:65:TYR:O	2.32	0.61
1:B:95:LYS:C	1:B:96:LYS:HG3	2.24	0.61
1:A:121:VAL:O	1:A:121:VAL:HG12	1.99	0.61
1:A:50:LEU:O	1:A:72:PHE:N	2.27	0.61
1:A:77:ASP:HB3	1:A:108:VAL:HB	1.82	0.61
1:B:81:ALA:HA	1:B:84:LEU:CB	2.31	0.61
1:B:97:VAL:O	1:B:100:PHE:HB2	2.00	0.61
1:A:7:ILE:HG22	1:A:8:TYR:N	2.14	0.60
1:A:111:LEU:HD23	1:A:114:LYS:CG	2.31	0.60
1:A:117:THR:O	1:A:120:GLN:HB2	2.00	0.60
1:A:51:LEU:C	1:A:71:SER:HG	2.09	0.60
1:A:70:SER:OG	1:A:71:SER:N	2.33	0.60
1:B:87:ILE:HA	1:B:91:TRP:CZ3	2.36	0.60
1:A:11:CYS:HB2	1:B:10:GLN:O	2.00	0.60
1:A:15:HIS:C	1:A:21:GLY:CA	2.61	0.60
1:A:37:LEU:O	1:A:37:LEU:HD23	2.01	0.60
1:B:26:PHE:CD1	1:B:26:PHE:N	2.64	0.60
1:A:117:THR:H	1:A:120:GLN:HB2	1.67	0.60
1:B:20:GLN:O	1:B:28:PRO:CB	2.49	0.60
1:A:77:ASP:OD1	1:A:109:LYS:N	2.35	0.60
1:A:22:ILE:O	1:A:22:ILE:HG23	2.02	0.59
1:A:32:HIS:CE1	1:A:60:VAL:HG13	2.37	0.59
1:B:31:GLY:O	1:B:33:VAL:N	2.36	0.59
1:A:76:LYS:O	1:A:78:GLU:C	2.46	0.59
1:A:75:LEU:HD12	1:A:80:ILE:CD1	2.33	0.59
1:B:79:GLU:O	1:B:82:ALA:CB	2.50	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:THR:C	1:A:119:GLN:H	2.11	0.58
1:B:7:ILE:HD12	1:B:82:ALA:CB	2.33	0.58
1:B:46:LEU:N	1:B:46:LEU:HD23	2.17	0.58
1:B:117:THR:O	1:B:120:GLN:HB2	2.03	0.58
1:A:6:LYS:O	1:A:9:ALA:CB	2.49	0.58
1:B:120:GLN:O	1:B:123:ALA:N	2.35	0.58
1:B:8:TYR:CE1	1:B:87:ILE:HG22	2.38	0.58
1:B:47:ILE:HD13	1:B:108:VAL:HG23	1.85	0.58
1:B:81:ALA:HA	1:B:84:LEU:HB3	1.86	0.58
1:A:6:LYS:HD2	1:A:6:LYS:N	2.18	0.58
1:B:4:GLY:N	1:B:6:LYS:CD	2.65	0.58
1:B:86:HIS:ND1	1:B:90:ALA:HB2	2.19	0.58
1:A:93:ASP:O	1:A:94:ALA:C	2.44	0.58
1:A:117:THR:H	1:A:120:GLN:HG3	1.69	0.58
1:B:123:ALA:C	1:B:125:ARG:N	2.58	0.58
1:A:76:LYS:O	1:A:78:GLU:N	2.36	0.58
1:B:17:GLN:HE21	1:B:17:GLN:N	2.01	0.58
1:B:76:LYS:HD3	1:B:79:GLU:OE1	2.04	0.58
1:A:89:THR:HG22	1:A:94:ALA:CB	2.29	0.57
1:B:16:GLN:C	1:B:17:GLN:NE2	2.60	0.57
1:B:82:ALA:C	1:B:85:ASN:H	2.11	0.57
1:A:100:PHE:O	1:A:102:PRO:HD3	2.04	0.57
1:B:93:ASP:O	1:B:96:LYS:HB2	2.05	0.57
1:A:79:GLU:O	1:A:80:ILE:O	2.23	0.57
1:A:116:LEU:HD22	1:A:120:GLN:NE2	2.18	0.57
1:B:25:ALA:C	1:B:26:PHE:HD1	2.12	0.57
1:B:51:LEU:HD21	1:B:112:ARG:HH22	1.68	0.57
1:B:94:ALA:CB	1:B:100:PHE:CE1	2.88	0.57
1:A:76:LYS:C	1:A:78:GLU:N	2.60	0.57
1:B:6:LYS:HD2	1:B:6:LYS:N	2.18	0.57
1:B:14:CYS:HA	1:B:26:PHE:CE2	2.40	0.57
1:B:123:ALA:O	1:B:124:GLU:C	2.47	0.57
1:A:78:GLU:O	1:A:79:GLU:C	2.47	0.57
1:B:83:VAL:CG2	2:B:200:HEC:CBC	2.82	0.56
1:B:78:GLU:O	1:B:79:GLU:C	2.48	0.56
1:A:22:ILE:N	1:A:23:PRO:CD	2.68	0.56
1:A:45:TYR:OH	1:A:125:ARG:HD2	2.04	0.56
1:B:94:ALA:HB2	1:B:100:PHE:CE1	2.39	0.56
1:B:116:LEU:O	1:B:117:THR:CG2	2.54	0.56
1:B:117:THR:HG1	1:B:120:GLN:HG3	1.70	0.56
1:B:119:GLN:O	1:B:123:ALA:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:ILE:O	1:B:22:ILE:CG1	2.51	0.56
1:B:48:LEU:CD2	1:B:52:TYR:CE2	2.80	0.56
1:B:83:VAL:HA	1:B:86:HIS:HB3	1.87	0.56
1:B:28:PRO:O	1:B:28:PRO:HG2	2.05	0.56
1:B:66:ASN:O	1:B:67:GLY:O	2.22	0.56
1:B:89:THR:OG1	1:B:90:ALA:N	2.37	0.56
1:A:72:PHE:CZ	1:B:12:ALA:HB3	2.41	0.56
1:A:83:VAL:HG13	1:A:83:VAL:O	2.05	0.56
1:A:41:GLY:HA2	1:A:44:GLU:CD	2.31	0.56
1:B:95:LYS:O	1:B:96:LYS:CG	2.49	0.56
1:B:9:ALA:C	1:B:11:CYS:N	2.63	0.56
1:B:93:ASP:HA	1:B:96:LYS:HE3	1.86	0.56
1:A:92:GLY:O	1:A:93:ASP:OD1	2.24	0.55
1:A:16:GLN:HB2	1:A:21:GLY:O	2.05	0.55
1:A:45:TYR:CE2	1:A:125:ARG:HD2	2.41	0.55
1:A:52:TYR:C	1:A:71:SER:HB2	2.31	0.55
1:B:76:LYS:N	1:B:76:LYS:CD	2.56	0.55
1:B:100:PHE:C	1:B:100:PHE:CD2	2.84	0.55
1:A:34:ALA:O	1:A:36:ILE:N	2.39	0.55
1:A:95:LYS:CG	1:A:96:LYS:N	2.39	0.55
1:B:4:GLY:N	1:B:6:LYS:HZ3	2.04	0.55
1:A:68:VAL:O	2:A:200:HEC:HMA1	2.07	0.55
1:A:80:ILE:C	1:A:82:ALA:N	2.61	0.55
1:A:84:LEU:C	1:A:86:HIS:H	2.14	0.55
1:A:77:ASP:OD2	1:A:109:LYS:CB	2.55	0.55
1:A:76:LYS:O	1:A:77:ASP:C	2.49	0.55
1:B:32:HIS:CG	1:B:32:HIS:O	2.60	0.55
1:B:16:GLN:HG3	1:B:21:GLY:H	1.70	0.54
1:B:32:HIS:HB2	1:B:61:LYS:HE2	1.90	0.54
1:B:98:LYS:C	1:B:100:PHE:N	2.63	0.54
1:A:119:GLN:O	1:A:120:GLN:C	2.51	0.54
1:A:22:ILE:O	1:A:23:PRO:C	2.51	0.54
1:B:50:LEU:HD21	2:B:200:HEC:CBC	2.38	0.54
1:B:60:VAL:C	1:B:62:GLY:N	2.61	0.54
1:A:103:PHE:O	1:A:104:THR:HG22	2.08	0.54
1:B:32:HIS:H	1:B:61:LYS:NZ	1.95	0.54
1:A:7:ILE:HD13	1:A:79:GLU:O	2.08	0.54
1:B:45:TYR:HA	1:B:48:LEU:CD1	2.23	0.54
1:B:116:LEU:C	1:B:117:THR:HG23	2.33	0.54
1:A:64:LYS:C	1:A:65:TYR:CD1	2.87	0.53
1:A:88:ALA:O	1:A:93:ASP:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:THR:C	1:A:119:GLN:N	2.65	0.53
1:B:28:PRO:O	1:B:32:HIS:HB3	2.08	0.53
1:B:29:LEU:O	1:B:33:VAL:HG23	2.07	0.53
1:A:113:ALA:O	1:A:115:LYS:N	2.41	0.53
1:A:11:CYS:SG	2:B:200:HEC:HBB1	2.48	0.53
1:B:39:LYS:HB3	1:B:128:LEU:CD2	2.38	0.53
1:B:83:VAL:O	1:B:84:LEU:C	2.51	0.53
1:B:103:PHE:O	1:B:105:ALA:N	2.42	0.53
1:B:31:GLY:O	1:B:93:ASP:OD2	2.26	0.53
1:B:82:ALA:O	1:B:83:VAL:C	2.51	0.53
1:A:37:LEU:HD12	1:A:46:LEU:CD1	2.38	0.53
1:A:60:VAL:O	1:A:61:LYS:C	2.52	0.53
1:A:58:ILE:HG13	1:A:125:ARG:HH12	1.74	0.53
1:A:68:VAL:HG23	1:A:69:MET:N	2.24	0.53
1:B:109:LYS:HA	1:B:112:ARG:HD3	1.89	0.53
1:A:80:ILE:HG23	1:A:84:LEU:HD11	1.91	0.53
1:B:18:ASN:OD1	1:B:20:GLN:HB3	2.09	0.53
1:B:68:VAL:O	1:B:68:VAL:CG2	2.45	0.53
1:A:32:HIS:O	1:A:33:VAL:C	2.45	0.52
1:B:22:ILE:HD12	1:B:23:PRO:CG	2.38	0.52
1:A:19:GLY:CA	1:A:91:TRP:CH2	2.92	0.52
1:B:71:SER:C	1:B:73:ALA:H	2.17	0.52
1:A:89:THR:O	1:A:91:TRP:N	2.34	0.52
1:A:31:GLY:HA2	1:A:93:ASP:OD1	2.08	0.52
1:B:8:TYR:CD1	1:B:87:ILE:HG22	2.45	0.52
1:B:14:CYS:HA	1:B:26:PHE:CD2	2.44	0.52
1:B:123:ALA:C	1:B:125:ARG:H	2.17	0.52
1:A:32:HIS:CD2	1:A:36:ILE:CD1	2.87	0.52
1:B:103:PHE:O	1:B:104:THR:C	2.53	0.52
1:A:31:GLY:O	1:A:34:ALA:N	2.36	0.52
1:A:59:GLU:CB	1:A:64:LYS:HG2	2.39	0.52
1:A:117:THR:H	1:A:120:GLN:CB	2.22	0.52
1:A:58:ILE:CB	1:A:125:ARG:NH1	2.73	0.51
1:B:44:GLU:HG3	1:B:111:LEU:CD1	2.37	0.51
1:B:101:LYS:HB3	1:B:102:PRO:CD	2.38	0.51
1:B:104:THR:O	1:B:105:ALA:C	2.52	0.51
1:A:121:VAL:O	1:A:122:LEU:C	2.46	0.51
1:A:86:HIS:CD2	1:A:90:ALA:HB3	2.45	0.51
1:A:52:TYR:HD2	1:A:116:LEU:HB2	1.74	0.51
1:A:72:PHE:CE1	1:B:12:ALA:HB3	2.46	0.51
1:A:80:ILE:CG2	1:A:81:ALA:H	2.04	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:ALA:C	1:B:96:LYS:H	2.19	0.51
1:B:104:THR:C	1:B:106:GLU:N	2.42	0.51
1:A:41:GLY:O	1:A:44:GLU:CA	2.59	0.51
1:A:84:LEU:O	1:A:88:ALA:N	2.44	0.51
1:B:42:GLY:O	1:B:46:LEU:CG	2.53	0.51
1:B:69:MET:HE1	2:B:200:HEC:C4C	2.41	0.51
1:B:108:VAL:HG13	1:B:112:ARG:CD	2.41	0.51
1:B:81:ALA:O	1:B:85:ASN:HB2	2.11	0.50
1:A:47:ILE:HG22	1:A:51:LEU:HD12	1.94	0.50
1:A:74:GLN:HG3	1:A:75:LEU:H	1.75	0.50
1:B:32:HIS:N	1:B:61:LYS:HZ3	2.08	0.50
1:A:7:ILE:C	1:A:9:ALA:N	2.67	0.50
1:A:15:HIS:O	1:A:21:GLY:CA	2.57	0.50
1:A:32:HIS:CA	1:A:35:GLU:OE2	2.46	0.50
1:A:95:LYS:O	1:A:96:LYS:C	2.54	0.50
1:A:74:GLN:HG3	1:A:75:LEU:N	2.26	0.50
1:A:30:ALA:C	1:A:32:HIS:H	2.20	0.50
1:B:59:GLU:OE2	1:B:62:GLY:CA	2.60	0.50
1:B:81:ALA:O	1:B:85:ASN:N	2.45	0.50
1:B:104:THR:O	1:B:107:GLU:N	2.44	0.50
1:B:108:VAL:HG13	1:B:112:ARG:CG	2.42	0.50
1:B:108:VAL:O	1:B:109:LYS:C	2.55	0.50
1:A:19:GLY:C	1:A:30:ALA:HB2	2.37	0.50
1:A:16:GLN:CB	1:A:21:GLY:O	2.60	0.50
1:A:80:ILE:CG2	1:A:84:LEU:HD11	2.41	0.50
1:A:111:LEU:O	1:A:114:LYS:HB2	2.12	0.50
1:B:25:ALA:C	1:B:26:PHE:CD1	2.90	0.49
1:B:35:GLU:CD	1:B:35:GLU:H	2.19	0.49
1:A:19:GLY:CA	1:A:91:TRP:CZ2	2.95	0.49
1:B:5:ALA:HA	1:B:86:HIS:CD2	2.47	0.49
1:B:108:VAL:HG13	1:B:112:ARG:HG3	1.93	0.49
1:A:50:LEU:O	1:A:71:SER:OG	2.30	0.49
1:B:22:ILE:HD12	1:B:22:ILE:C	2.38	0.49
1:A:28:PRO:O	1:A:32:HIS:HB3	2.12	0.49
1:B:17:GLN:N	1:B:17:GLN:NE2	2.60	0.49
1:A:61:LYS:O	1:A:63:MET:N	2.43	0.49
1:A:14:CYS:HA	1:A:26:PHE:CE2	2.47	0.49
1:B:50:LEU:HD12	1:B:72:PHE:HB2	1.94	0.49
1:B:57:GLN:HG2	1:B:66:ASN:HB2	1.94	0.49
1:A:22:ILE:O	1:A:22:ILE:CG2	2.60	0.49
1:A:56:GLY:O	1:A:58:ILE:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:LEU:HB3	1:A:103:PHE:CE1	2.48	0.49
1:A:87:ILE:HD12	2:A:200:HEC:HAC	1.93	0.49
1:A:41:GLY:O	1:A:44:GLU:CB	2.61	0.49
1:A:123:ALA:O	1:A:126:LYS:HB3	2.13	0.49
1:A:113:ALA:O	1:A:114:LYS:C	2.54	0.49
1:A:50:LEU:HD11	2:A:200:HEC:HBC3	1.95	0.48
1:A:35:GLU:OE2	1:A:61:LYS:HE3	2.13	0.48
1:B:14:CYS:O	1:B:26:PHE:HD2	1.96	0.48
1:B:94:ALA:HA	1:B:100:PHE:CE1	2.49	0.48
1:A:13:GLY:O	1:A:15:HIS:N	2.46	0.48
1:B:60:VAL:HG12	1:B:63:MET:N	2.28	0.48
1:A:74:GLN:CG	1:A:75:LEU:H	2.26	0.48
1:A:80:ILE:CG2	1:A:81:ALA:N	2.57	0.48
1:A:129:GLY:O	1:A:130:LEU:HG	2.13	0.48
1:B:33:VAL:O	1:B:33:VAL:HG12	2.14	0.48
1:B:55:GLN:CG	1:B:118:PRO:CB	2.69	0.48
1:B:86:HIS:O	1:B:90:ALA:CB	2.62	0.48
1:A:77:ASP:HB3	1:A:105:ALA:O	2.13	0.48
1:B:18:ASN:OD1	1:B:20:GLN:CB	2.62	0.48
1:B:69:MET:O	1:B:70:SER:C	2.56	0.48
1:A:107:GLU:HA	1:A:110:LYS:HB3	1.96	0.48
1:A:113:ALA:C	1:A:115:LYS:N	2.71	0.48
1:B:81:ALA:HA	1:B:84:LEU:HB2	1.95	0.48
1:A:26:PHE:HE2	2:A:200:HEC:HMB1	1.78	0.47
1:B:44:GLU:HB3	1:B:111:LEU:CD2	2.38	0.47
1:A:34:ALA:HB1	1:A:97:VAL:HG23	1.95	0.47
1:A:51:LEU:HD21	1:A:112:ARG:CD	2.43	0.47
1:B:65:TYR:N	1:B:65:TYR:CD1	2.82	0.47
1:A:119:GLN:O	1:A:122:LEU:N	2.48	0.47
1:B:7:ILE:C	1:B:9:ALA:N	2.72	0.47
1:B:45:TYR:O	1:B:49:VAL:N	2.37	0.47
1:A:7:ILE:C	1:A:9:ALA:H	2.21	0.47
1:A:39:LYS:NZ	1:A:130:LEU:C	2.73	0.47
1:A:57:GLN:HB2	1:A:66:ASN:OD1	2.14	0.47
1:B:7:ILE:CD1	1:B:82:ALA:HB3	2.44	0.47
1:B:22:ILE:HD12	1:B:23:PRO:HG2	1.95	0.47
1:A:53:GLY:O	1:A:121:VAL:HG21	2.13	0.47
1:A:83:VAL:O	1:A:87:ILE:HG23	2.15	0.47
1:A:95:LYS:HG3	1:A:96:LYS:CG	2.45	0.47
1:A:117:THR:H	1:A:120:GLN:CG	2.27	0.47
1:A:50:LEU:CD1	2:A:200:HEC:HBC3	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:ASN:O	1:B:89:THR:CG2	2.50	0.47
1:B:45:TYR:HE1	1:B:121:VAL:HG12	1.79	0.47
1:B:119:GLN:O	1:B:122:LEU:N	2.48	0.47
1:A:22:ILE:HG22	1:A:26:PHE:CD1	2.48	0.46
1:B:41:GLY:HA3	1:B:128:LEU:HD11	1.97	0.46
1:A:15:HIS:CA	1:A:21:GLY:HA2	2.41	0.46
1:B:103:PHE:N	1:B:103:PHE:CD1	2.83	0.46
1:A:35:GLU:H	1:A:35:GLU:HG3	1.50	0.46
1:A:58:ILE:CG1	1:A:125:ARG:HH12	2.29	0.46
1:A:85:ASN:N	1:A:103:PHE:CD1	2.82	0.46
1:A:18:ASN:ND2	1:A:20:GLN:CB	2.76	0.46
1:A:77:ASP:O	1:A:81:ALA:HB2	2.15	0.46
1:A:74:GLN:O	1:A:75:LEU:C	2.58	0.46
1:B:83:VAL:O	1:B:86:HIS:N	2.48	0.46
1:A:94:ALA:CB	1:A:100:PHE:HE2	2.29	0.46
1:B:119:GLN:O	1:B:122:LEU:CB	2.62	0.46
1:B:121:VAL:HG12	1:B:121:VAL:O	2.14	0.46
1:B:127:LYS:C	1:B:129:GLY:N	2.74	0.46
1:A:85:ASN:CG	1:A:103:PHE:HD1	2.23	0.46
1:B:60:VAL:C	1:B:62:GLY:H	2.22	0.46
1:B:117:THR:OG1	1:B:120:GLN:CG	2.52	0.46
1:A:74:GLN:CG	1:A:75:LEU:N	2.78	0.45
1:A:85:ASN:ND2	1:A:103:PHE:N	2.58	0.45
1:B:4:GLY:O	1:B:86:HIS:HB2	2.17	0.45
1:B:36:ILE:HG22	1:B:42:GLY:CA	2.47	0.45
1:B:41:GLY:N	1:B:128:LEU:HD21	2.32	0.45
1:A:56:GLY:O	1:A:57:GLN:O	2.34	0.45
1:B:39:LYS:HB3	1:B:128:LEU:HD23	1.98	0.45
1:A:19:GLY:C	1:A:21:GLY:N	2.70	0.45
1:A:77:ASP:C	1:A:78:GLU:O	2.59	0.45
1:A:111:LEU:C	1:A:113:ALA:N	2.74	0.45
1:B:81:ALA:HB1	1:B:103:PHE:CB	2.47	0.45
1:B:122:LEU:HD12	1:B:122:LEU:HA	1.61	0.45
1:A:109:LYS:HA	1:A:112:ARG:HG2	1.99	0.45
1:A:51:LEU:CA	1:A:73:ALA:HB2	2.46	0.45
1:B:104:THR:OG1	1:B:107:GLU:HB2	2.17	0.45
1:B:86:HIS:CE1	1:B:90:ALA:HB2	2.51	0.45
2:B:200:HEC:HMD1	2:B:200:HEC:HBD2	1.98	0.45
1:A:16:GLN:HE21	1:A:16:GLN:H	1.55	0.44
1:A:81:ALA:O	1:A:103:PHE:HB2	2.17	0.44
1:B:55:GLN:CD	1:B:118:PRO:HB3	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:GLY:HA2	1:A:93:ASP:OD2	2.17	0.44
1:B:113:ALA:C	1:B:115:LYS:H	2.22	0.44
1:B:117:THR:HB	1:B:118:PRO:HD2	1.98	0.44
1:A:32:HIS:ND1	1:A:60:VAL:HG13	2.32	0.44
1:A:54:LEU:CD1	1:A:122:LEU:HD13	2.46	0.44
1:A:78:GLU:O	1:A:80:ILE:C	2.60	0.44
1:B:86:HIS:C	1:B:88:ALA:N	2.72	0.44
1:B:16:GLN:HG2	1:B:21:GLY:H	1.82	0.44
1:B:100:PHE:CD2	1:B:101:LYS:N	2.85	0.44
1:A:45:TYR:CZ	1:A:125:ARG:HD2	2.53	0.44
1:A:51:LEU:C	1:A:73:ALA:HB2	2.43	0.44
1:A:77:ASP:CA	1:A:108:VAL:HG11	2.35	0.44
1:A:86:HIS:O	1:A:90:ALA:HB3	2.17	0.44
1:B:41:GLY:C	1:B:43:ARG:H	2.24	0.44
1:B:45:TYR:O	1:B:48:LEU:CA	2.66	0.44
1:A:71:SER:HG	1:A:73:ALA:HB2	1.82	0.44
1:A:75:LEU:HB2	1:A:80:ILE:CD1	2.43	0.44
1:B:8:TYR:CB	1:B:86:HIS:HD2	2.31	0.44
1:B:28:PRO:O	1:B:32:HIS:CB	2.66	0.44
1:B:44:GLU:HG2	1:B:111:LEU:CD2	2.45	0.43
1:A:84:LEU:O	1:A:87:ILE:N	2.51	0.43
1:B:114:LYS:O	1:B:115:LYS:HB2	2.18	0.43
1:A:4:GLY:HA2	1:A:7:ILE:HD12	2.01	0.43
1:A:33:VAL:O	1:A:37:LEU:HB2	2.18	0.43
1:A:103:PHE:C	1:A:104:THR:CG2	2.90	0.43
1:B:54:LEU:HD23	2:B:200:HEC:HBA1	2.01	0.43
1:B:108:VAL:C	1:B:110:LYS:H	2.25	0.43
1:A:109:LYS:C	1:A:111:LEU:H	2.27	0.43
1:B:14:CYS:SG	2:B:200:HEC:CMB	3.06	0.43
1:A:16:GLN:HB2	1:A:21:GLY:C	2.44	0.43
1:A:76:LYS:H	1:A:76:LYS:HD3	1.84	0.43
1:B:44:GLU:CG	1:B:111:LEU:HD11	2.41	0.43
1:A:37:LEU:O	1:A:38:ALA:O	2.36	0.43
1:B:37:LEU:HD23	1:B:37:LEU:HA	1.78	0.43
1:A:81:ALA:O	1:A:85:ASN:OD1	2.37	0.43
1:B:101:LYS:HB3	1:B:101:LYS:HE3	1.69	0.43
1:A:34:ALA:C	1:A:36:ILE:N	2.75	0.43
1:B:22:ILE:C	1:B:23:PRO:O	2.61	0.43
1:B:78:GLU:HA	1:B:105:ALA:HB1	2.01	0.43
1:A:88:ALA:O	1:A:93:ASP:CB	2.67	0.42
1:B:38:ALA:O	1:B:39:LYS:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:GLN:O	1:B:122:LEU:HD22	2.19	0.42
1:B:13:GLY:O	1:B:14:CYS:HB2	2.18	0.42
1:B:56:GLY:HA3	1:B:122:LEU:CD2	2.45	0.42
1:B:117:THR:O	1:B:118:PRO:C	2.62	0.42
1:A:16:GLN:HB3	1:A:18:ASN:OD1	2.19	0.42
1:A:13:GLY:O	1:A:14:CYS:HB2	2.18	0.42
1:A:15:HIS:HA	1:A:21:GLY:CA	2.50	0.42
1:B:28:PRO:HD3	1:B:60:VAL:HG21	1.98	0.42
1:B:7:ILE:CG2	1:B:83:VAL:HG12	2.47	0.42
1:B:45:TYR:CE1	1:B:49:VAL:HG22	2.54	0.42
1:B:60:VAL:O	1:B:62:GLY:N	2.53	0.42
1:A:69:MET:HG2	1:A:70:SER:O	2.20	0.41
1:B:36:ILE:CG2	1:B:42:GLY:HA2	2.49	0.41
1:B:47:ILE:O	1:B:51:LEU:N	2.43	0.41
1:A:45:TYR:CD1	1:A:45:TYR:C	2.93	0.41
1:B:28:PRO:O	1:B:28:PRO:CG	2.67	0.41
1:B:85:ASN:HA	1:B:88:ALA:CB	2.49	0.41
1:B:93:ASP:HA	1:B:96:LYS:HE2	2.02	0.41
1:B:100:PHE:C	1:B:100:PHE:HD2	2.28	0.41
1:A:66:ASN:C	2:A:200:HEC:O2A	2.63	0.41
1:A:106:GLU:O	1:A:110:LYS:N	2.49	0.41
1:B:36:ILE:HG22	1:B:42:GLY:O	2.20	0.41
1:A:4:GLY:O	1:A:86:HIS:HB2	2.20	0.41
1:A:114:LYS:O	1:A:116:LEU:CD2	2.61	0.41
1:B:94:ALA:HA	1:B:100:PHE:CD1	2.55	0.41
1:A:31:GLY:HA2	1:A:93:ASP:CG	2.46	0.41
1:A:38:ALA:O	1:A:39:LYS:C	2.63	0.41
1:A:63:MET:CE	1:A:63:MET:HB3	2.50	0.41
1:B:14:CYS:C	1:B:16:GLN:H	2.28	0.41
1:B:48:LEU:O	1:B:52:TYR:N	2.27	0.41
1:A:117:THR:OG1	1:A:120:GLN:HG2	2.17	0.41
1:B:7:ILE:C	1:B:9:ALA:H	2.28	0.41
1:B:46:LEU:O	1:B:50:LEU:HB2	2.20	0.41
1:A:109:LYS:C	1:A:111:LEU:N	2.76	0.41
1:B:26:PHE:N	1:B:26:PHE:HD1	2.11	0.41
1:B:29:LEU:O	1:B:30:ALA:C	2.64	0.41
1:B:59:GLU:OE2	1:B:62:GLY:HA2	2.20	0.41
1:B:85:ASN:CA	1:B:88:ALA:HB3	2.51	0.41
1:B:92:GLY:CA	1:B:95:LYS:HG2	2.51	0.41
1:A:13:GLY:O	1:A:14:CYS:C	2.63	0.41
1:A:58:ILE:CG1	1:A:125:ARG:NH1	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:ALA:O	2:B:200:HEC:HMA2	2.21	0.41
1:B:35:GLU:O	1:B:36:ILE:C	2.61	0.41
1:B:54:LEU:C	1:B:55:GLN:CG	2.92	0.41
1:B:45:TYR:O	1:B:46:LEU:C	2.62	0.41
1:A:20:GLN:O	1:A:23:PRO:HD2	2.20	0.40
1:A:52:TYR:O	1:A:118:PRO:HD3	2.21	0.40
1:B:60:VAL:HG12	1:B:63:MET:H	1.86	0.40
1:B:99:GLY:O	1:B:101:LYS:HG2	2.21	0.40
1:A:59:GLU:HA	1:A:64:LYS:HA	2.03	0.40
1:A:75:LEU:CB	1:A:79:GLU:CB	2.91	0.40
1:A:90:ALA:O	1:A:91:TRP:CG	2.72	0.40
1:B:9:ALA:O	1:B:10:GLN:C	2.64	0.40
1:B:22:ILE:HA	1:B:23:PRO:HD2	1.78	0.40
1:B:50:LEU:HD13	1:B:50:LEU:HA	1.84	0.40
1:B:60:VAL:O	1:B:61:LYS:C	2.65	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	126/132 (96%)	72 (57%)	19 (15%)	35 (28%)	0	0
1	B	126/132 (96%)	69 (55%)	35 (28%)	22 (18%)	0	0
All	All	252/264 (96%)	141 (56%)	54 (21%)	57 (23%)	0	0

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	38	ALA
1	A	73	ALA

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Mol	Chain	Res	Type
1	A	78	GLU
1	A	79	GLU
1	A	80	ILE
1	A	81	ALA
1	A	83	VAL
1	A	90	ALA
1	A	96	LYS
1	A	99	GLY
1	A	118	PRO
1	B	5	ALA
1	B	10	GLN
1	B	23	PRO
1	B	24	GLY
1	B	32	HIS
1	B	45	TYR
1	B	70	SER
1	B	105	ALA
1	B	107	GLU
1	B	114	LYS
1	B	116	LEU
1	B	128	LEU
1	A	5	ALA
1	A	47	ILE
1	A	49	VAL
1	A	57	GLN
1	A	62	GLY
1	A	67	GLY
1	A	77	ASP
1	A	91	TRP
1	A	95	LYS
1	A	114	LYS
1	B	14	CYS
1	B	42	GLY
1	B	67	GLY
1	B	104	THR
1	B	113	ALA
1	B	124	GLU
1	A	23	PRO
1	A	35	GLU
1	A	39	LYS
1	A	48	LEU
1	A	94	ALA

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Mol	Chain	Res	Type
1	A	102	PRO
1	A	115	LYS
1	B	127	LYS
1	A	30	ALA
1	A	130	LEU
1	B	96	LYS
1	A	8	TYR
1	A	127	LYS
1	B	80	ILE
1	B	118	PRO
1	A	42	GLY
1	A	31	GLY

5.3.2 Protein sidechains ⓘ

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	96/99 (97%)	70 (73%)	26 (27%)	0	2
1	B	96/99 (97%)	81 (84%)	15 (16%)	2	13
All	All	192/198 (97%)	151 (79%)	41 (21%)	1	6

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	18	ASN
1	A	22	ILE
1	A	23	PRO
1	A	33	VAL
1	A	35	GLU
1	A	37	LEU
1	A	40	GLU
1	A	50	LEU
1	A	51	LEU
1	A	58	ILE

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Mol	Chain	Res	Type
1	A	68	VAL
1	A	70	SER
1	A	75	LEU
1	A	80	ILE
1	A	85	ASN
1	A	86	HIS
1	A	87	ILE
1	A	93	ASP
1	A	102	PRO
1	A	104	THR
1	A	111	LEU
1	A	116	LEU
1	A	119	GLN
1	A	125	ARG
1	A	126	LYS
1	B	28	PRO
1	B	36	ILE
1	B	39	LYS
1	B	47	ILE
1	B	50	LEU
1	B	63	MET
1	B	70	SER
1	B	83	VAL
1	B	84	LEU
1	B	87	ILE
1	B	102	PRO
1	B	108	VAL
1	B	119	GLN
1	B	128	LEU
1	B	130	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	85	ASN
1	A	86	HIS
1	A	119	GLN
1	A	120	GLN
1	B	16	GLN
1	B	17	GLN
1	B	85	ASN

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Mol	Chain	Res	Type
1	B	86	HIS
1	B	119	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	A	200	1	50,50,50	2.91	30 (60%)	68,82,82	1.75	11 (16%)
2	HEC	B	200	1	50,50,50	3.35	27 (54%)	68,82,82	1.70	13 (19%)

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	A	200	1	1/1/3/7	7/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEC	B	200	1	1/1/3/7	9/14/54/54	-

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	200	HEC	C1A-NA	-7.75	1.25	1.39
2	B	200	HEC	C4A-C3A	-7.71	1.30	1.45
2	B	200	HEC	C1A-C2A	-6.91	1.33	1.45
2	A	200	HEC	C1D-ND	-6.67	1.28	1.40
2	B	200	HEC	CAB-C3B	-6.58	1.34	1.51
2	B	200	HEC	CAC-C3C	-6.19	1.35	1.51
2	B	200	HEC	C4A-NA	-5.85	1.28	1.39
2	B	200	HEC	C4C-C3C	-5.68	1.33	1.44
2	A	200	HEC	C1B-NB	-5.63	1.27	1.38
2	B	200	HEC	C4D-ND	-5.54	1.28	1.38
2	A	200	HEC	CAC-C3C	-5.43	1.37	1.51
2	A	200	HEC	CBD-CGD	5.39	1.63	1.50
2	A	200	HEC	C4A-C3A	-4.92	1.35	1.45
2	A	200	HEC	C4B-NB	-4.82	1.31	1.40
2	B	200	HEC	C4B-NB	-4.79	1.32	1.40
2	B	200	HEC	C1D-ND	-4.41	1.32	1.40
2	A	200	HEC	C1A-C2A	-4.39	1.37	1.45
2	A	200	HEC	C4A-NA	-4.00	1.32	1.39
2	B	200	HEC	C1C-NC	-3.96	1.32	1.39
2	A	200	HEC	FE-NC	3.86	2.07	1.95
2	B	200	HEC	CHC-C1C	3.75	1.47	1.39
2	A	200	HEC	C4D-C3D	-3.72	1.38	1.45
2	B	200	HEC	FE-NA	3.71	2.07	1.95
2	A	200	HEC	C4C-NC	-3.70	1.32	1.39
2	A	200	HEC	CHD-C1D	-3.55	1.31	1.38
2	A	200	HEC	C1D-C2D	-3.54	1.37	1.44
2	A	200	HEC	FE-NA	3.50	2.06	1.95
2	B	200	HEC	FE-ND	3.28	2.05	1.94
2	A	200	HEC	FE-NB	3.04	2.04	1.94
2	A	200	HEC	C1A-NA	-3.03	1.33	1.39
2	B	200	HEC	CHB-C1B	3.01	1.46	1.39
2	B	200	HEC	FE-NC	2.98	2.05	1.95
2	A	200	HEC	CHB-C4A	-2.97	1.32	1.38
2	B	200	HEC	C1D-C2D	-2.89	1.38	1.44
2	A	200	HEC	C1C-NC	-2.88	1.34	1.39
2	B	200	HEC	C2A-C3A	-2.82	1.30	1.36
2	A	200	HEC	C2A-C3A	2.81	1.42	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	200	HEC	FE-NB	2.78	2.03	1.94
2	B	200	HEC	CBB-CAB	-2.72	1.40	1.51
2	B	200	HEC	C4D-C3D	-2.69	1.40	1.45
2	A	200	HEC	CBB-CAB	-2.67	1.40	1.51
2	A	200	HEC	O2A-CGA	-2.65	1.22	1.30
2	B	200	HEC	CBC-CAC	-2.60	1.40	1.51
2	A	200	HEC	CAB-C3B	-2.55	1.44	1.51
2	A	200	HEC	CMA-C3A	-2.53	1.45	1.50
2	B	200	HEC	CHD-C1D	-2.52	1.33	1.38
2	A	200	HEC	C4D-ND	-2.49	1.34	1.38
2	A	200	HEC	C3C-C2C	-2.39	1.32	1.38
2	A	200	HEC	CBC-CAC	-2.37	1.41	1.51
2	B	200	HEC	CHC-C4B	2.32	1.43	1.38
2	B	200	HEC	CAD-C3D	2.30	1.57	1.51
2	A	200	HEC	CBA-CGA	2.29	1.55	1.50
2	A	200	HEC	O1D-CGD	2.18	1.29	1.22
2	B	200	HEC	C1B-C2B	-2.14	1.40	1.44
2	A	200	HEC	C4B-C3B	-2.12	1.41	1.45
2	A	200	HEC	CHB-C1B	2.10	1.44	1.39
2	B	200	HEC	C4C-NC	-2.04	1.35	1.39

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	200	HEC	CBC-CAC-C3C	6.24	129.34	112.42
2	B	200	HEC	CBC-CAC-C3C	6.02	128.73	112.42
2	A	200	HEC	CBB-CAB-C3B	5.88	128.35	112.42
2	B	200	HEC	CBB-CAB-C3B	5.46	127.23	112.42
2	A	200	HEC	C4B-NB-C1B	3.26	109.07	105.21
2	B	200	HEC	O2A-CGA-CBA	3.10	123.78	114.00
2	B	200	HEC	CHC-C4B-NB	-3.02	120.63	124.37
2	B	200	HEC	O1A-CGA-CBA	-2.83	114.13	123.09
2	B	200	HEC	CHC-C4B-C3B	2.76	130.31	125.23
2	A	200	HEC	O2A-CGA-O1A	-2.66	116.48	123.33
2	A	200	HEC	C4A-CHB-C1B	2.63	131.61	126.02
2	A	200	HEC	O2A-CGA-CBA	2.58	122.14	114.00
2	B	200	HEC	C1D-C2D-C3D	-2.54	104.31	106.98
2	A	200	HEC	CAC-C3C-C2C	2.51	130.86	126.89
2	B	200	HEC	CAC-C3C-C2C	2.46	130.79	126.89
2	B	200	HEC	C1A-CHA-C4D	2.43	131.18	126.02
2	A	200	HEC	C1A-C2A-C3A	-2.36	104.00	107.11
2	A	200	HEC	CAB-C3B-C2B	2.26	131.70	127.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	200	HEC	CMD-C2D-C1D	2.08	128.28	125.03
2	A	200	HEC	CBD-CAD-C3D	2.07	118.27	112.53
2	A	200	HEC	CHB-C4A-NA	-2.07	122.20	124.45
2	B	200	HEC	CMB-C2B-C3B	2.03	131.63	126.15
2	B	200	HEC	C4A-CHB-C1B	2.03	130.32	126.02
2	B	200	HEC	CAC-C3C-C4C	-2.02	122.13	124.91

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	200	HEC	NA
2	B	200	HEC	NA

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	200	HEC	C2C-C3C-CAC-CBC
2	B	200	HEC	C2C-C3C-CAC-CBC
2	B	200	HEC	C2D-C3D-CAD-CBD
2	B	200	HEC	C4C-C3C-CAC-CBC
2	A	200	HEC	C2B-C3B-CAB-CBB
2	A	200	HEC	C4C-C3C-CAC-CBC
2	A	200	HEC	C4B-C3B-CAB-CBB
2	B	200	HEC	C4D-C3D-CAD-CBD
2	A	200	HEC	C2A-CAA-CBA-CGA
2	B	200	HEC	C2A-CAA-CBA-CGA
2	B	200	HEC	CAD-CBD-CGD-O1D
2	A	200	HEC	CAA-CBA-CGA-O1A
2	B	200	HEC	CAD-CBD-CGD-O2D
2	A	200	HEC	CAA-CBA-CGA-O2A
2	B	200	HEC	CAA-CBA-CGA-O2A
2	B	200	HEC	CAA-CBA-CGA-O1A

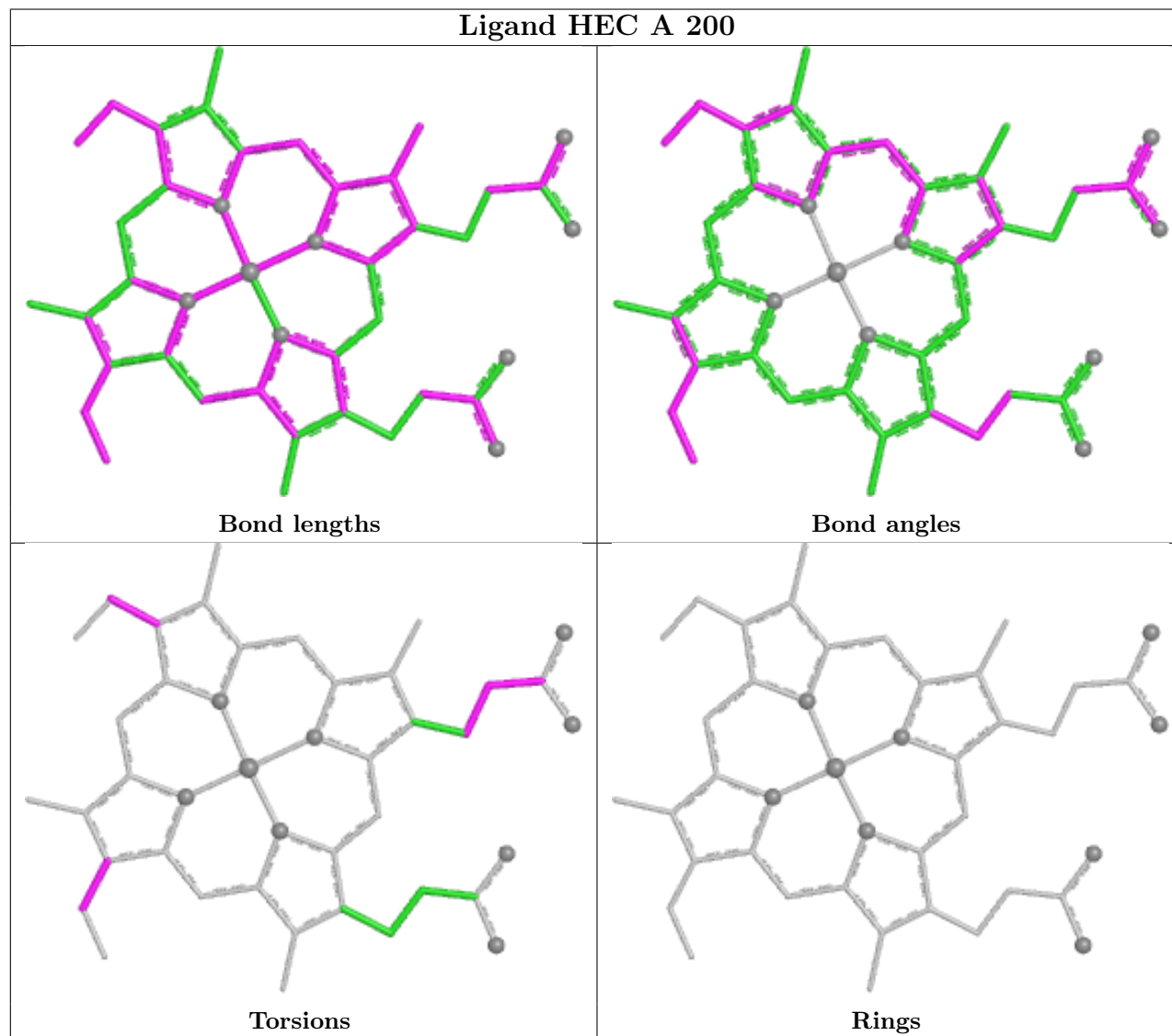
There are no ring outliers.

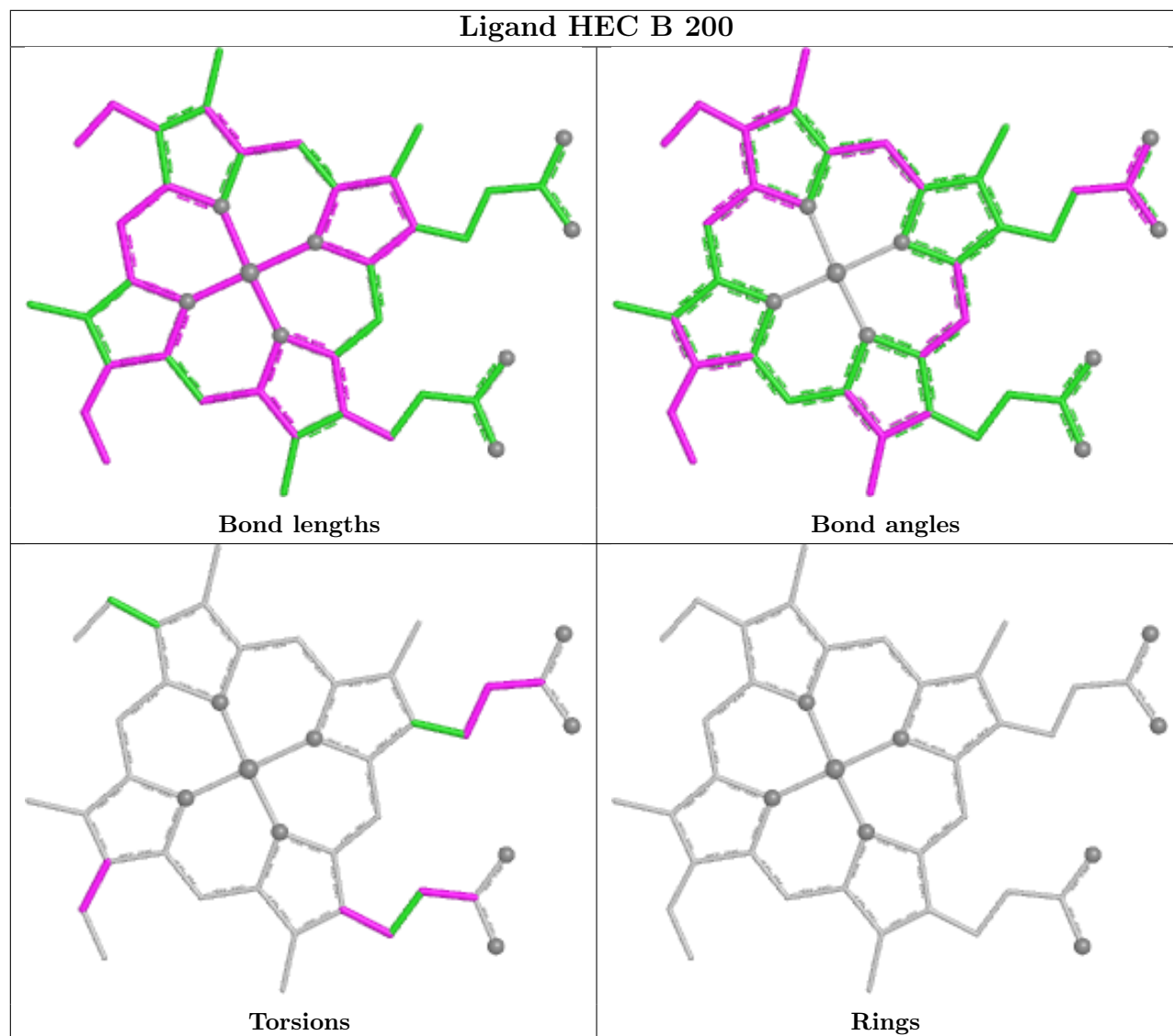
2 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	200	HEC	7	0
2	B	200	HEC	14	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 than 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.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	128/132 (96%)	0.17	2 (1%)	70 47	9, 75, 108, 138	8 (6%)
1	B	128/132 (96%)	0.18	3 (2%)	61 38	8, 73, 112, 149	8 (6%)
All	All	256/264 (96%)	0.18	5 (1%)	65 41	8, 75, 109, 149	16 (6%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	103	PHE	3.1
1	A	25	ALA	2.8
1	B	58	ILE	2.7
1	A	44	GLU	2.2
1	B	99	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

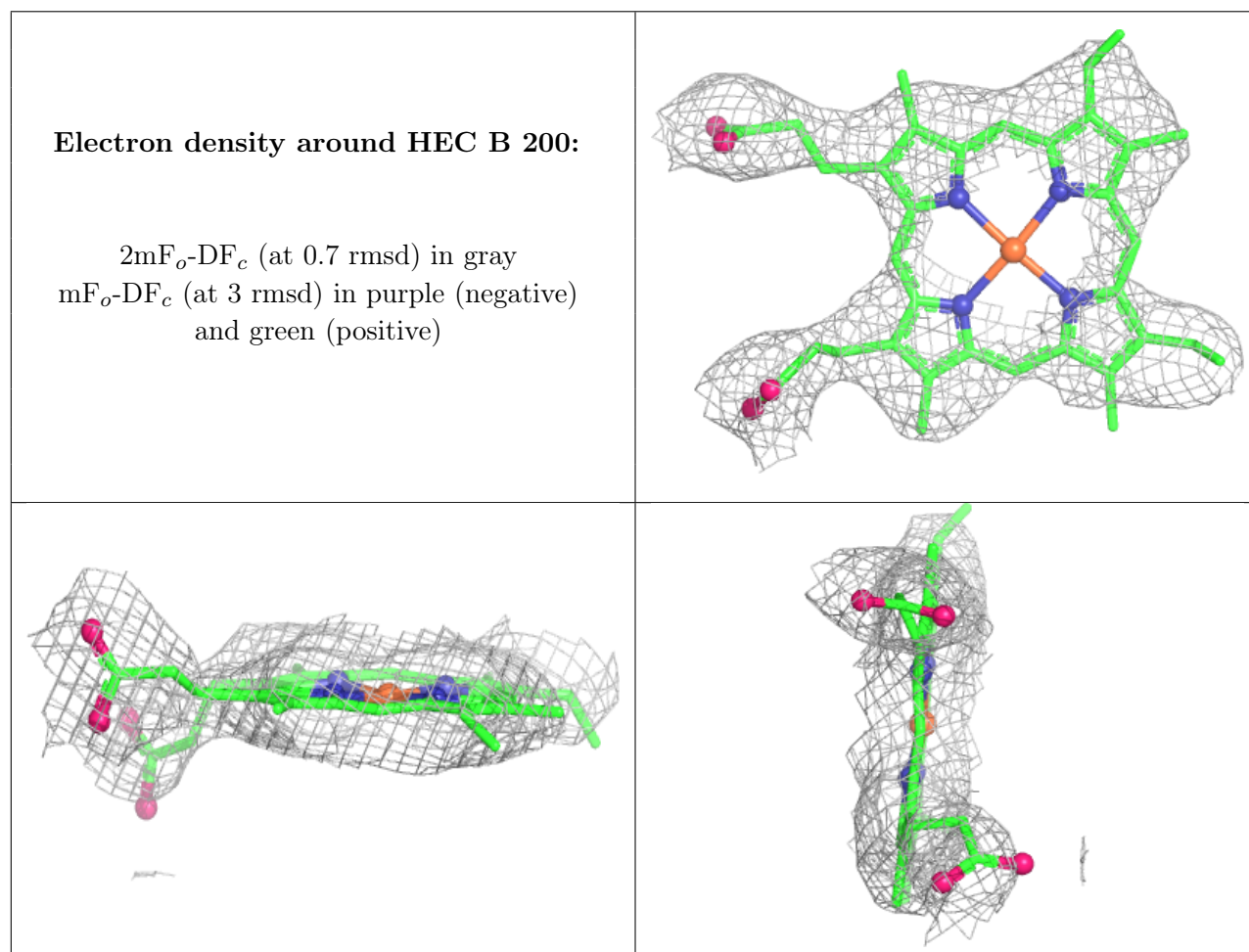
There are no oligosaccharides in this entry.

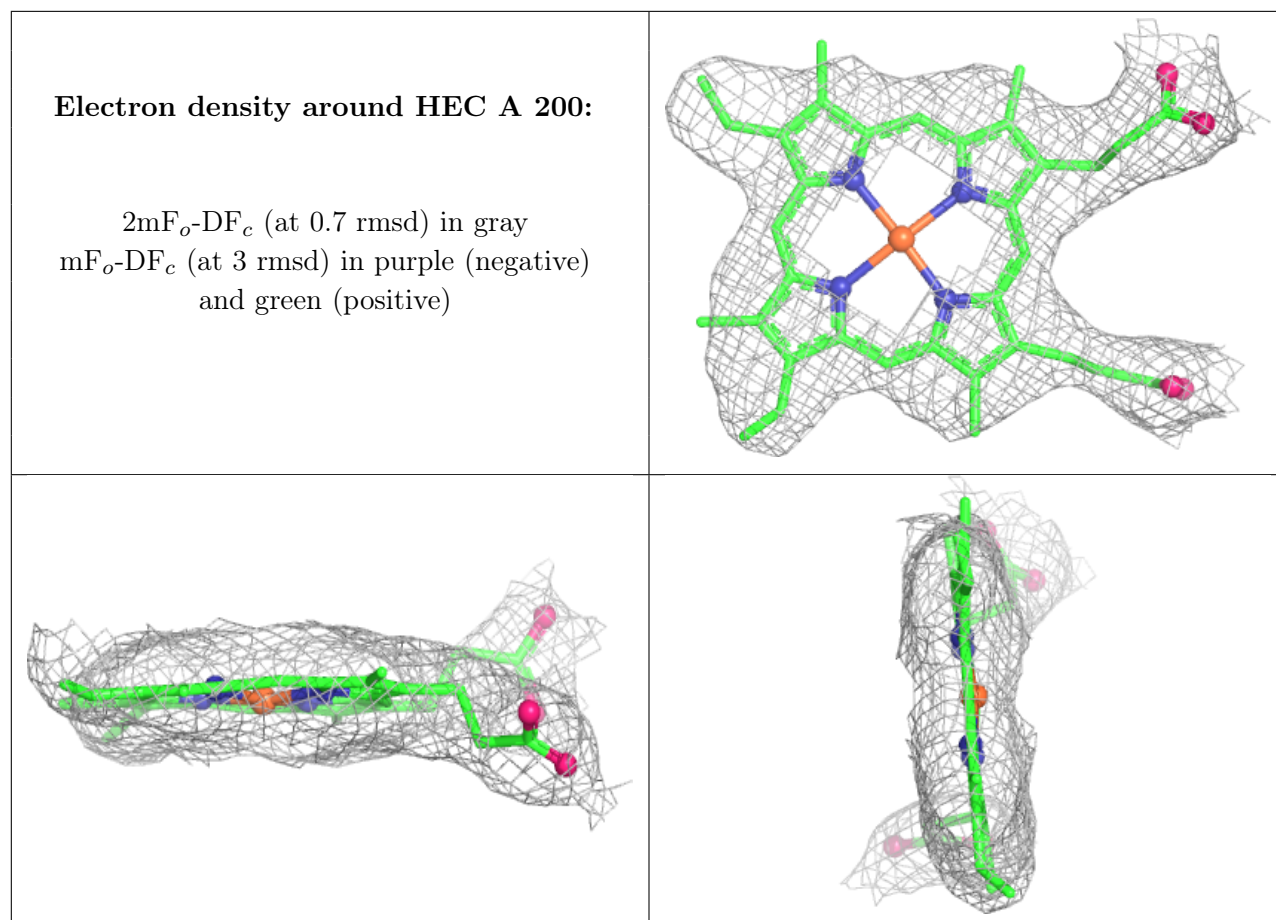
6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	HEC	B	200	43/43	0.94	0.09	36,49,64,68	0
2	HEC	A	200	43/43	0.96	0.07	4,34,50,59	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





6.5 Other polymers ⓘ

There are no such residues in this entry.