Full wwPDB X-ray Structure Validation Report (i)

Jul 18, 2016 – 01:22 PM EDT

PDB ID	:	5DJQ
Title	:	The structure of CBB3 cytochrome oxidase.
Authors	:	Buschmann, S.; Warkentin, E.; Xie, H.; Kohlstaedt, M.; Langer, J.D.; Ermler, U.; Michel, H.
Deposited on	:	2015-09-02
Resolution	:	3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

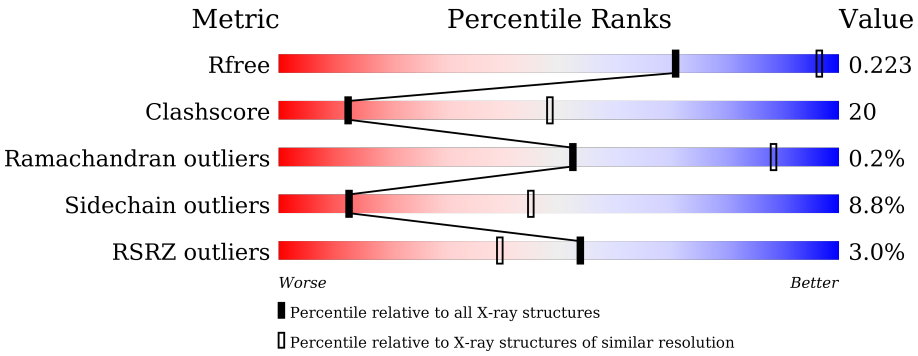
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027790
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027790

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 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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

Mol	Chain	Length	Quality of chain
1	A	474	64% 30%
1	D	474	4% 61% 34%
1	G	474	60% 34%
1	K	474	3% 63% 31%
2	B	203	67% 26%
2	E	203	3% 68% 26%

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Mol	Chain	Length	Quality of chain
2	H	203	69% 25%
2	L	203	3% 71% 23%
3	C	311	% 61% 33%
3	F	311	7% 50% 37% 9%
3	I	311	2% 59% 31% 7%
3	M	311	5% 56% 36% 5%
4	N	36	6% 56% 22% 19%
4	O	36	19% 53% 25% 19%
4	P	36	3% 44% 33% 19%
4	Q	36	8% 50% 22% 6% 19%

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
11	FC6	F	403	-	-	-	X
9	PO4	K	506	-	-	X	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 31974 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 Cbb3-type cytochrome c oxidase subunit CcoN1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	466	Total	C	N	O	S	0	0	0
			3683	2461	593	607	22			
1	D	463	Total	C	N	O	S	0	0	0
			3663	2450	590	601	22			
1	G	465	Total	C	N	O	S	0	0	0
			3676	2457	592	605	22			
1	K	465	Total	C	N	O	S	0	0	0
			3676	2457	592	605	22			

- Molecule 2 is a protein called Cbb3-type cytochrome c oxidase subunit II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	197	Total	C	N	O	S	0	0	0
			1548	981	268	289	10			
2	E	197	Total	C	N	O	S	0	0	0
			1548	981	268	289	10			
2	H	197	Total	C	N	O	S	0	0	0
			1548	981	268	289	10			
2	L	197	Total	C	N	O	S	0	0	0
			1548	981	268	289	10			

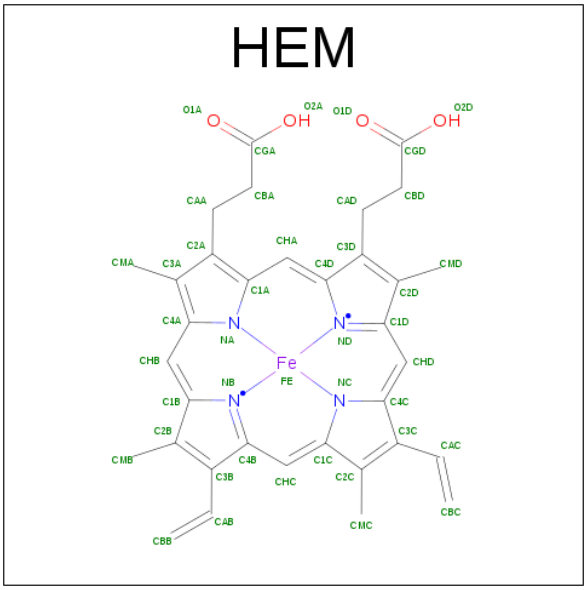
- Molecule 3 is a protein called Cbb3-type cytochrome c oxidase subunit CcoP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	303	Total	C	N	O	S	0	0	0
			2312	1483	391	427	11			
3	F	303	Total	C	N	O	S	0	0	0
			2312	1483	391	427	11			
3	I	303	Total	C	N	O	S	0	0	0
			2312	1483	391	427	11			
3	M	303	Total	C	N	O	S	0	0	0
			2312	1483	391	427	11			

- Molecule 4 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	N	29	Total	C	N	O	S	0	0	0
			221	154	31	34	2			
4	O	29	Total	C	N	O	S	0	0	0
			221	154	31	34	2			
4	P	29	Total	C	N	O	S	0	0	0
			221	154	31	34	2			
4	Q	29	Total	C	N	O	S	0	0	0
			221	154	31	34	2			

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	G	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	G	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	K	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	K	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

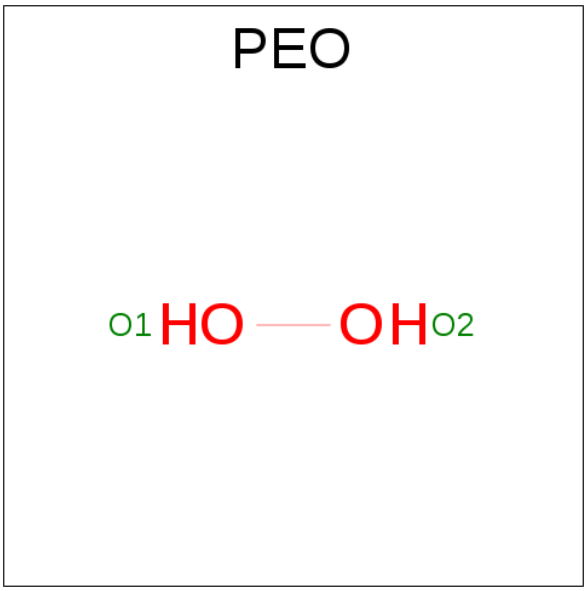
- Molecule 6 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	1	Total	Cu	0	0
			1	1		
6	A	1	Total	Cu	0	0
			1	1		
6	D	1	Total	Cu	0	0
			1	1		
6	K	1	Total	Cu	0	0
			1	1		

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

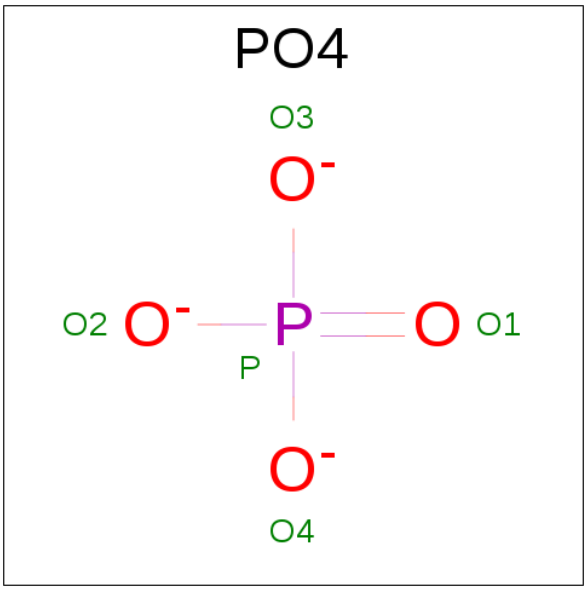
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	G	2	Total	Ca	0	0
			2	2		
7	A	2	Total	Ca	0	0
			2	2		
7	D	2	Total	Ca	0	0
			2	2		
7	K	2	Total	Ca	0	0
			2	2		

- Molecule 8 is HYDROGEN PEROXIDE (three-letter code: PEO) (formula: H_2O_2).



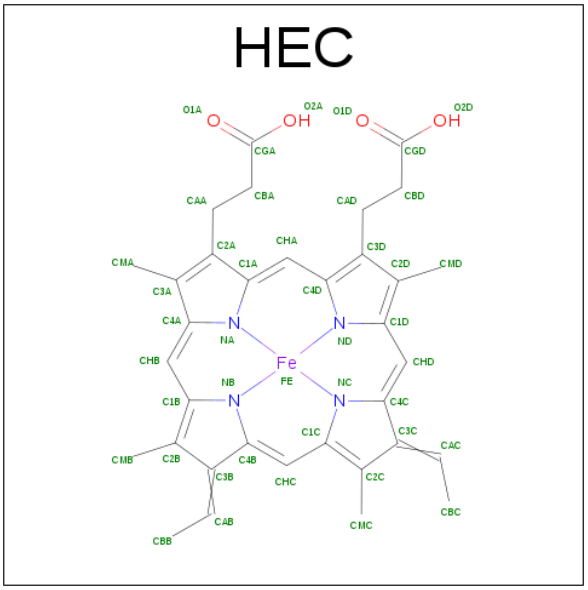
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total O 2 2	0	0
8	D	1	Total O 2 2	0	0
8	G	1	Total O 2 2	0	0
8	K	1	Total O 2 2	0	0

- Molecule 9 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total O P 5 4 1	0	0
9	D	1	Total O P 5 4 1	0	0
9	G	1	Total O P 5 4 1	0	0
9	K	1	Total O P 5 4 1	0	0

- Molecule 10 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	B	1	Total C Fe N O 43 34 1 4 4	0	0
10	C	1	Total C Fe N O 43 34 1 4 4	0	0
10	C	1	Total C Fe N O 43 34 1 4 4	0	0
10	E	1	Total C Fe N O 43 34 1 4 4	0	0
10	F	1	Total C Fe N O 43 34 1 4 4	0	0
10	F	1	Total C Fe N O 43 34 1 4 4	0	0
10	H	1	Total C Fe N O 43 34 1 4 4	0	0
10	I	1	Total C Fe N O 43 34 1 4 4	0	0

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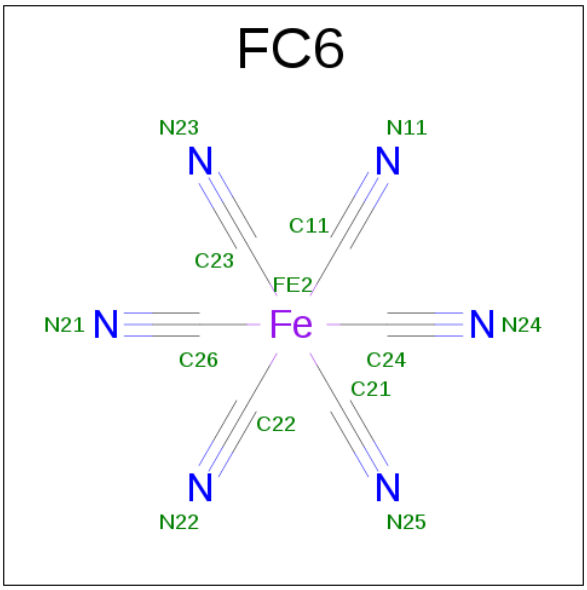
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	I	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
10	L	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
10	M	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
10	M	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 11 is HEXACYANOFERRATE(3-) (three-letter code: FC6) (formula: C_6FeN_6).

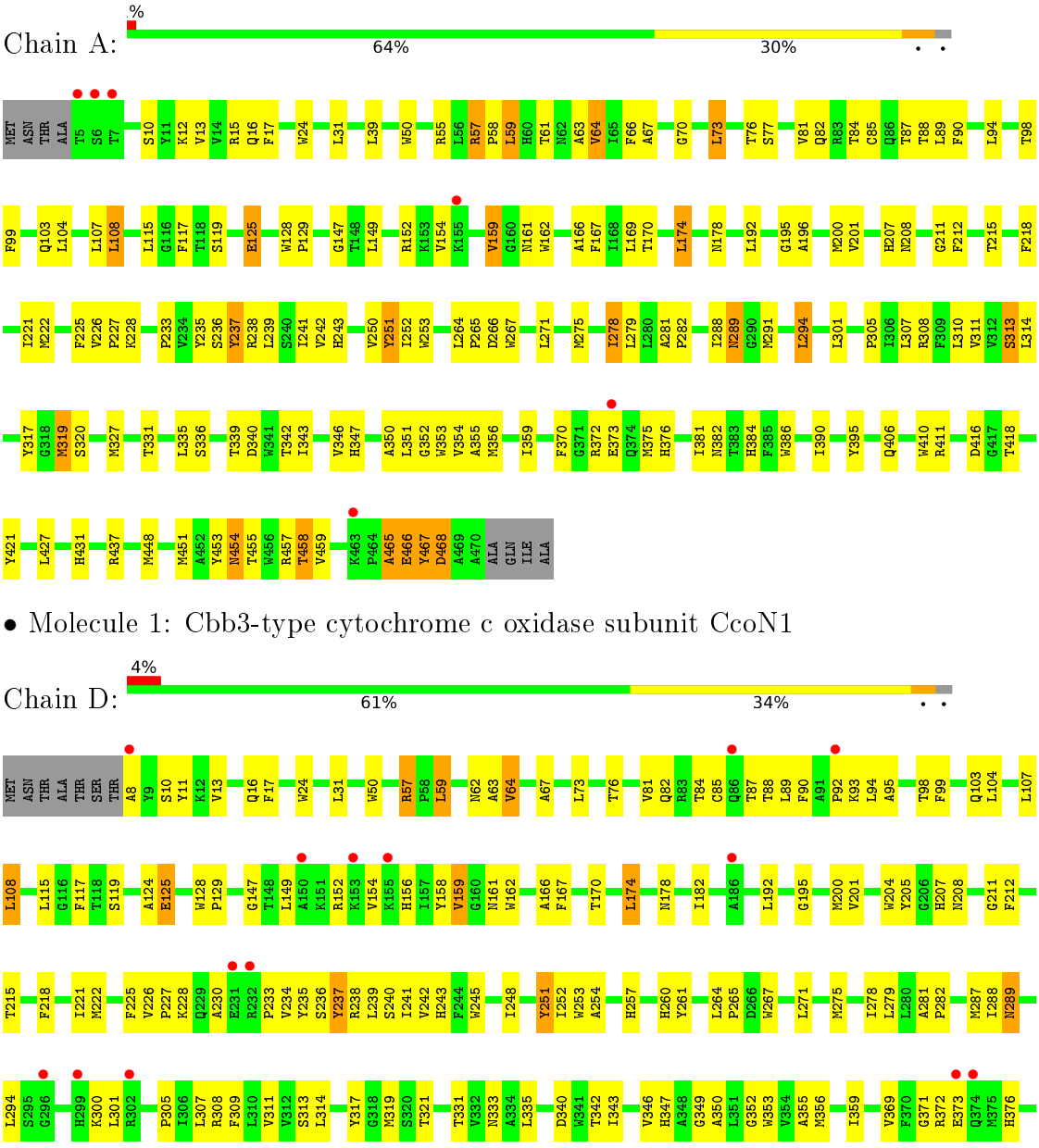


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	C	1	Total	C	Fe	N	0	0
			13	6	1	6		
11	F	1	Total	C	Fe	N	0	0
			13	6	1	6		
11	I	1	Total	C	Fe	N	0	0
			13	6	1	6		
11	M	1	Total	C	Fe	N	0	0
			13	6	1	6		

3 Residue-property plots (i)

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

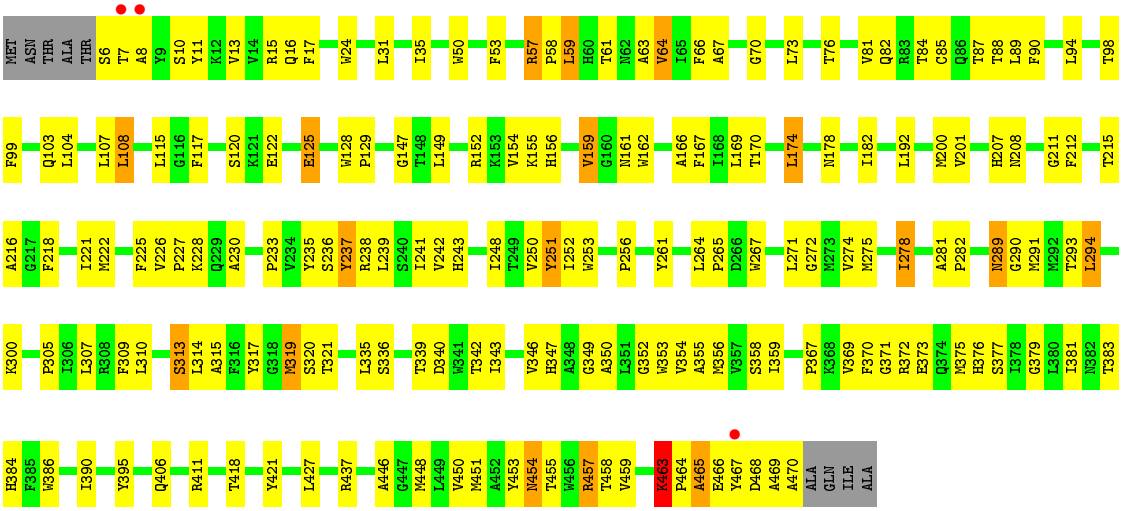
- Molecule 1: Cbb3-type cytochrome c oxidase subunit CcoN1



- Molecule 1: Cbb3-type cytochrome c oxidase subunit CcoN1

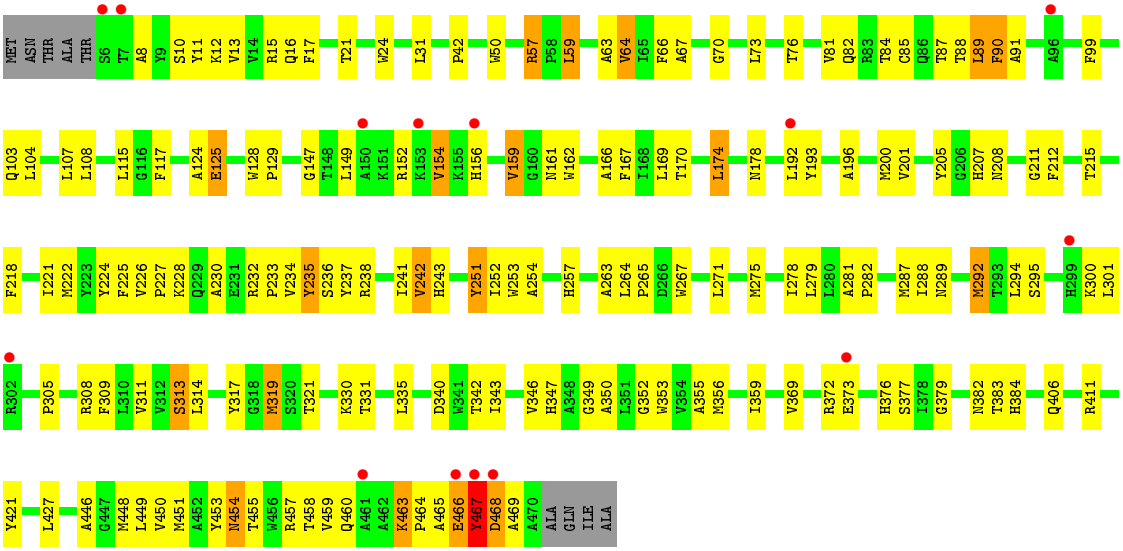
• Molecule 1: Cbb3-type cytochrome c oxidase subunit CcoN1

Chain G:



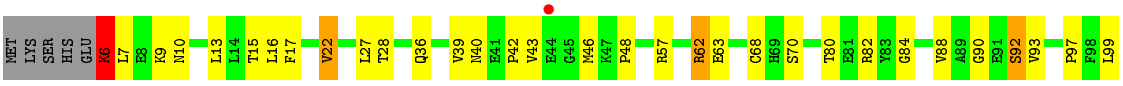
• Molecule 1: Cbb3-type cytochrome c oxidase subunit CcoN1

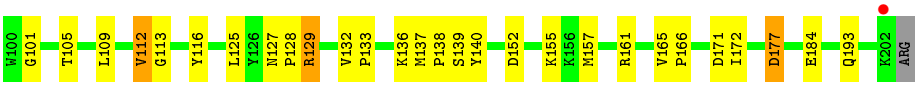
Chain K:



• Molecule 2: Cbb3-type cytochrome c oxidase subunit II

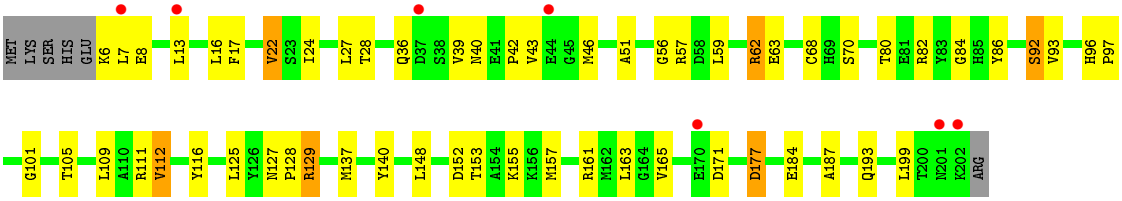
Chain B:





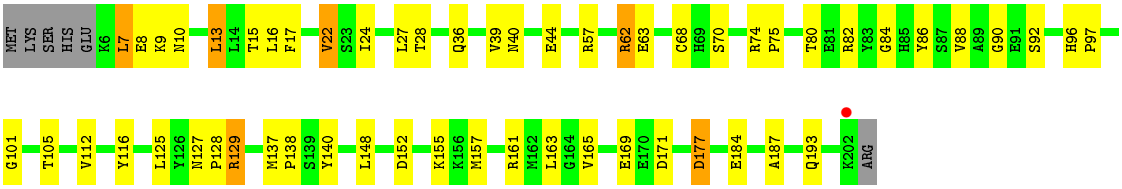
• Molecule 2: Cbb3-type cytochrome c oxidase subunit II

Chain E:



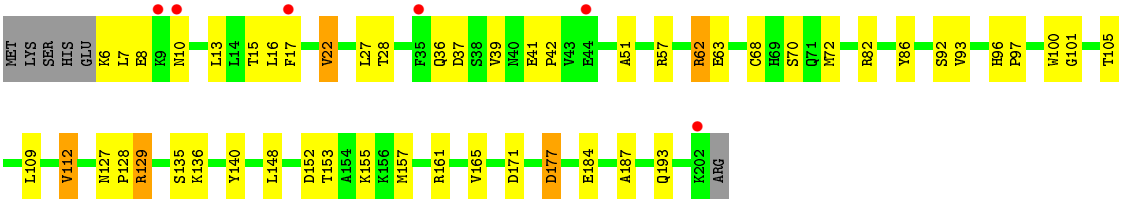
• Molecule 2: Cbb3-type cytochrome c oxidase subunit II

Chain H:



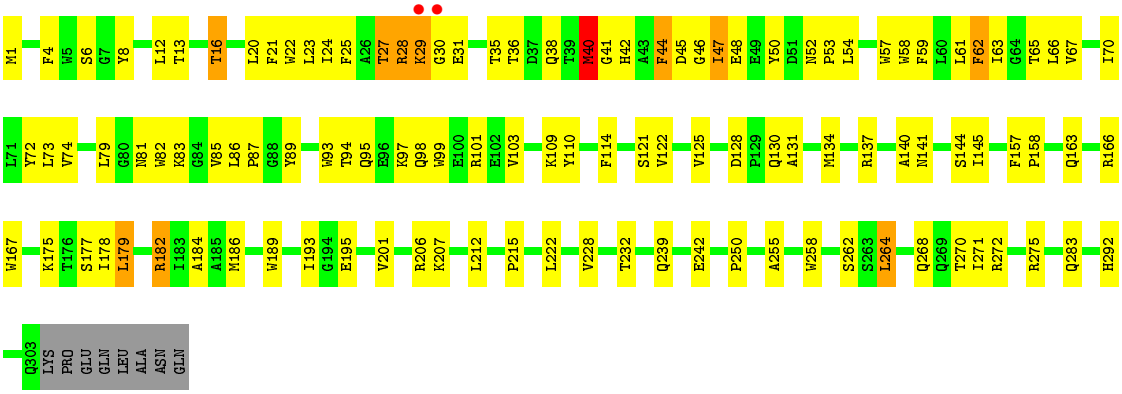
• Molecule 2: Cbb3-type cytochrome c oxidase subunit II

Chain L:



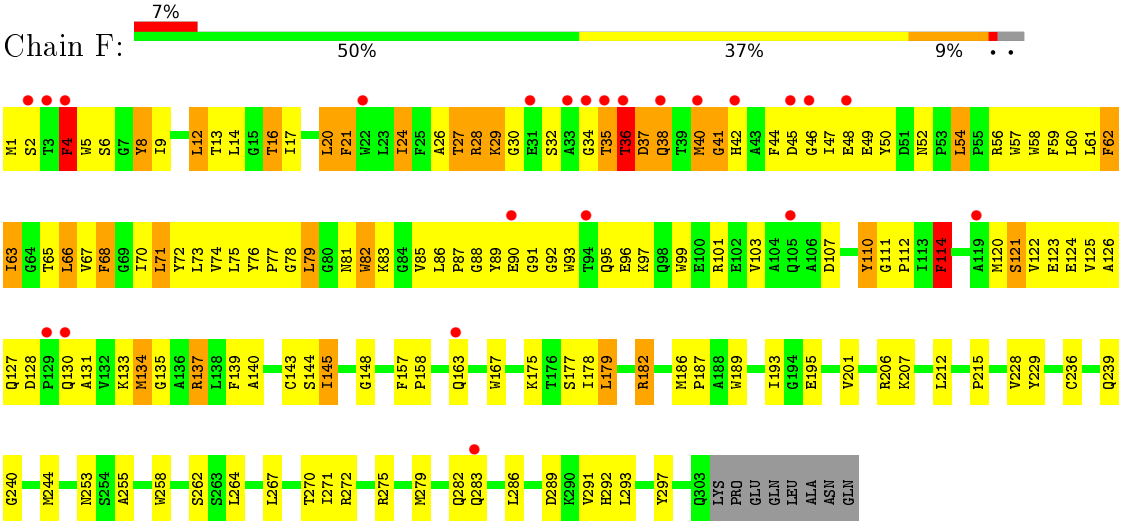
• Molecule 3: Cbb3-type cytochrome c oxidase subunit CcoP1

Chain C:



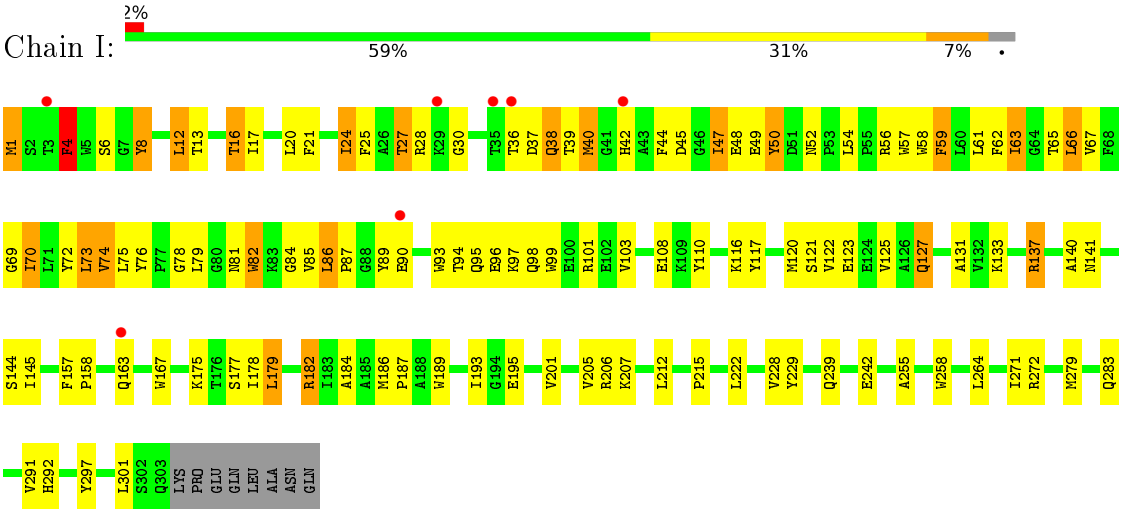
• Molecule 3: Cbb3-type cytochrome c oxidase subunit CcoP1

Chain F:



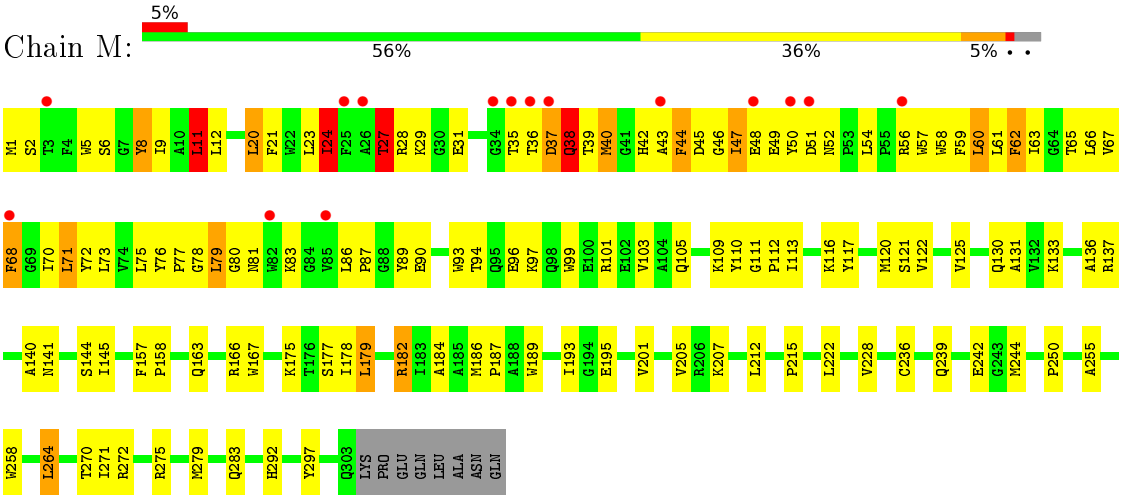
• Molecule 3: Cbb3-type cytochrome c oxidase subunit CcoP1

Chain I:



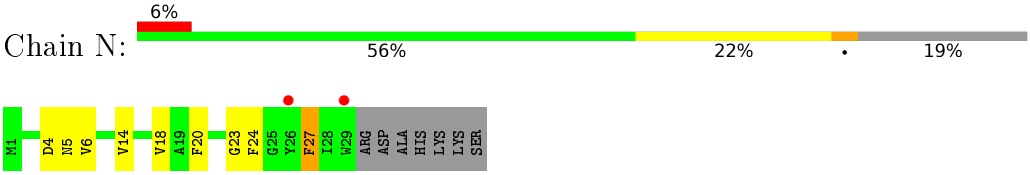
• Molecule 3: Cbb3-type cytochrome c oxidase subunit CcoP1

Chain M:



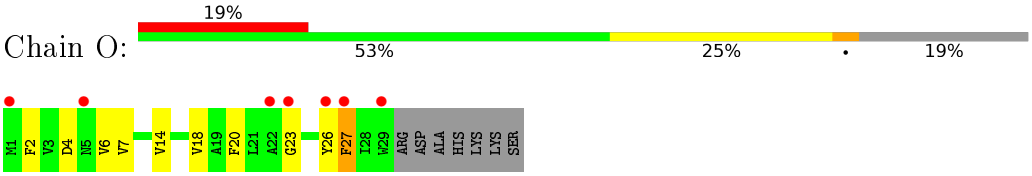
- Molecule 4: Putative uncharacterized protein

Chain N:



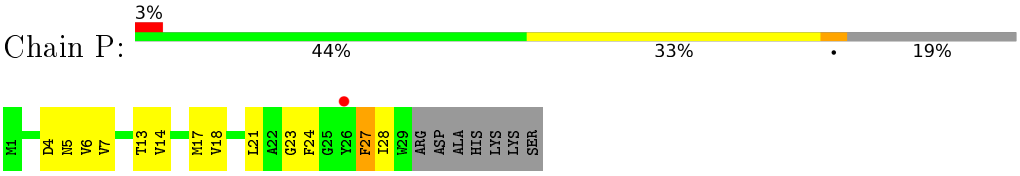
- Molecule 4: Putative uncharacterized protein

Chain O:



- Molecule 4: Putative uncharacterized protein

Chain P:



- Molecule 4: Putative uncharacterized protein

Chain Q:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	136.47Å 279.93Å 175.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.98 – 3.20 14.98 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.5 (14.98-3.20) 98.8 (14.98-3.00)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	1.69 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.187 , 0.223 0.187 , 0.223	Depositor DCC
R_{free} test set	5482 reflections (5.06%)	DCC
Wilson B-factor (Å^2)	86.4	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 72.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	31974	wwPDB-VP
Average B, all atoms (Å^2)	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.95% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FC6, CA, PEO, HEC, HEM, PO4, CU

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	0.39	0/3811	0.64	5/5210 (0.1%)
1	D	0.36	0/3791	0.66	9/5182 (0.2%)
1	G	0.40	1/3804 (0.0%)	0.60	4/5200 (0.1%)
1	K	0.37	0/3804	0.60	4/5200 (0.1%)
2	B	0.38	0/1584	0.60	1/2146 (0.0%)
2	E	0.30	0/1584	0.53	0/2146
2	H	0.34	0/1584	0.57	0/2146
2	L	0.31	0/1584	0.52	0/2146
3	C	0.50	0/2374	0.89	9/3225 (0.3%)
3	F	0.56	2/2374 (0.1%)	1.02	10/3225 (0.3%)
3	I	0.54	1/2374 (0.0%)	0.91	12/3225 (0.4%)
3	M	0.54	0/2374	0.89	5/3225 (0.2%)
4	N	0.50	0/227	0.85	2/309 (0.6%)
4	O	0.47	0/227	0.82	2/309 (0.6%)
4	P	0.50	0/227	0.89	2/309 (0.6%)
4	Q	0.65	0/227	0.96	2/309 (0.6%)
All	All	0.43	4/31950 (0.0%)	0.73	67/43512 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	G	0	1
3	C	0	1
3	F	0	2
3	I	0	2
All	All	0	8

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	110	TYR	CD2-CE2	-8.28	1.26	1.39
3	I	82	TRP	CB-CG	-7.12	1.37	1.50
3	F	110	TYR	CE2-CZ	-5.39	1.31	1.38
1	G	237	TYR	CD2-CE2	-5.10	1.31	1.39

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	44	PHE	CB-CG-CD1	-10.56	113.41	120.80
3	I	44	PHE	CB-CG-CD1	-10.03	113.78	120.80
3	F	66	LEU	CB-CG-CD1	-9.58	94.72	111.00
3	M	79	LEU	CB-CG-CD1	-9.16	95.42	111.00
1	D	462	ALA	N-CA-C	8.96	135.18	111.00
1	A	468	ASP	N-CA-C	-8.90	86.96	111.00
3	F	110	TYR	CB-CG-CD2	-8.84	115.69	121.00
1	A	467	TYR	N-CA-C	-8.59	87.81	111.00
3	C	41	GLY	N-CA-C	8.35	133.97	113.10
3	C	28	ARG	CB-CA-C	-8.08	94.24	110.40
4	P	27	PHE	CB-CG-CD1	-8.05	115.17	120.80
3	I	44	PHE	CB-CG-CD2	8.03	126.42	120.80
3	F	110	TYR	CB-CG-CD1	7.90	125.74	121.00
1	G	237	TYR	CB-CG-CD2	-7.89	116.26	121.00
3	M	24	ILE	CG1-CB-CG2	-7.88	94.06	111.40
4	N	27	PHE	CB-CG-CD1	-7.82	115.33	120.80
4	Q	27	PHE	CB-CG-CD1	-7.81	115.33	120.80
3	F	79	LEU	CB-CG-CD1	-7.73	97.86	111.00
4	O	27	PHE	CB-CG-CD1	-7.53	115.53	120.80
4	P	27	PHE	CB-CG-CD2	7.50	126.05	120.80
1	A	467	TYR	C-N-CA	7.40	140.19	121.70
1	A	467	TYR	CA-C-N	-7.18	101.39	117.20
4	N	27	PHE	CB-CG-CD2	6.80	125.56	120.80
1	G	237	TYR	CB-CG-CD1	6.79	125.07	121.00
3	C	42	HIS	N-CA-CB	6.77	122.78	110.60
1	D	457	ARG	NE-CZ-NH1	-6.70	116.95	120.30
3	I	28	ARG	CB-CA-C	-6.61	97.18	110.40
1	D	457	ARG	CG-CD-NE	6.58	125.61	111.80
4	O	27	PHE	CB-CG-CD2	6.57	125.40	120.80
1	D	456	TRP	CB-CG-CD1	-6.55	118.48	127.00
1	D	457	ARG	NE-CZ-NH2	6.44	123.52	120.30
1	D	462	ALA	N-CA-CB	-6.40	101.14	110.10
3	I	4	PHE	CB-CG-CD2	-6.33	116.37	120.80
3	I	1	MET	CB-CA-C	-6.32	97.75	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	110	TYR	CB-CG-CD1	-6.32	117.21	121.00
1	K	292	MET	CA-CB-CG	6.29	124.00	113.30
3	C	42	HIS	N-CA-C	-6.21	94.22	111.00
2	B	6	LYS	CD-CE-NZ	-5.91	98.11	111.70
3	F	36	THR	OG1-CB-CG2	5.83	123.41	110.00
3	C	40	MET	C-N-CA	-5.83	110.06	122.30
1	K	242	VAL	CB-CA-C	-5.76	100.45	111.40
1	G	457	ARG	CD-NE-CZ	5.76	131.66	123.60
3	F	41	GLY	C-N-CA	-5.75	107.33	121.70
3	F	4	PHE	CB-CG-CD2	-5.71	116.80	120.80
1	D	457	ARG	CD-NE-CZ	-5.70	115.62	123.60
1	D	468	ASP	N-CA-C	-5.62	95.84	111.00
3	C	29	LYS	N-CA-C	5.59	126.08	111.00
3	C	44	PHE	N-CA-C	-5.58	95.93	111.00
3	M	11	LEU	CA-CB-CG	5.57	128.10	115.30
3	C	44	PHE	CB-CG-CD2	5.46	124.62	120.80
3	I	59	PHE	CB-CG-CD1	-5.45	116.99	120.80
3	F	114	PHE	CB-CG-CD2	-5.43	117.00	120.80
1	K	467	TYR	N-CA-C	5.40	125.58	111.00
3	M	47	ILE	CG1-CB-CG2	-5.38	99.56	111.40
3	I	50	TYR	CA-CB-CG	5.38	123.62	113.40
4	Q	27	PHE	CB-CG-CD2	5.37	124.56	120.80
1	K	463	LYS	C-N-CD	-5.32	108.89	120.60
3	I	70	ILE	CG1-CB-CG2	-5.31	99.72	111.40
3	F	66	LEU	CB-CG-CD2	5.30	120.00	111.00
3	I	4	PHE	CB-CG-CD1	5.29	124.50	120.80
1	D	237	TYR	CB-CG-CD2	5.20	124.12	121.00
3	F	56	ARG	CB-CG-CD	5.18	125.08	111.60
1	A	237	TYR	CB-CG-CD2	-5.17	117.90	121.00
3	I	82	TRP	CB-CG-CD2	-5.14	119.92	126.60
1	G	463	LYS	O-C-N	-5.08	111.44	121.10
3	M	27	THR	CA-CB-CG2	-5.08	105.28	112.40
3	I	110	TYR	CB-CG-CD2	5.08	124.05	121.00

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	465	ALA	Mainchain
1	A	467	TYR	Peptide
3	C	44	PHE	Sidechain
3	F	114	PHE	Sidechain

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Mol	Chain	Res	Type	Group
3	F	37	ASP	Peptide
1	G	463	LYS	Mainchain
3	I	4	PHE	Sidechain
3	I	74	VAL	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3683	0	3663	134	0
1	D	3663	0	3644	161	0
1	G	3676	0	3656	150	0
1	K	3676	0	3656	158	0
2	B	1548	0	1526	46	0
2	E	1548	0	1526	48	0
2	H	1548	0	1526	42	0
2	L	1548	0	1526	39	0
3	C	2312	0	2237	103	0
3	F	2312	0	2237	194	0
3	I	2312	0	2237	124	0
3	M	2312	0	2237	147	0
4	N	221	0	226	9	0
4	O	221	0	226	11	0
4	P	221	0	226	12	0
4	Q	221	0	226	12	0
5	A	86	0	60	12	0
5	D	86	0	60	13	0
5	G	86	0	60	13	0
5	K	86	0	60	13	0
6	A	1	0	0	0	0
6	D	1	0	0	0	0
6	G	1	0	0	0	0
6	K	1	0	0	0	0
7	A	2	0	0	0	0
7	D	2	0	0	0	0
7	G	2	0	0	0	0
7	K	2	0	0	0	0
8	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	D	2	0	0	0	0
8	G	2	0	0	0	0
8	K	2	0	0	0	0
9	A	5	0	0	1	0
9	D	5	0	0	1	0
9	G	5	0	0	1	0
9	K	5	0	0	4	0
10	B	43	0	30	5	0
10	C	86	0	60	11	0
10	E	43	0	30	6	0
10	F	86	0	60	10	0
10	H	43	0	30	6	0
10	I	86	0	60	11	0
10	L	43	0	30	4	0
10	M	86	0	60	11	0
11	C	13	0	0	2	0
11	F	13	0	0	2	0
11	I	13	0	0	1	0
11	M	13	0	0	2	0
All	All	31974	0	31175	1240	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 20.

All (1240) 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:D:207:HIS:NE2	1:D:251:TYR:CE1	1.70	1.59
1:A:207:HIS:NE2	1:A:251:TYR:CE1	1.70	1.56
1:G:207:HIS:NE2	1:G:251:TYR:CE1	1.70	1.56
1:K:207:HIS:NE2	1:K:251:TYR:CE1	1.70	1.53
1:K:207:HIS:NE2	1:K:251:TYR:HE1	1.02	1.33
1:D:207:HIS:NE2	1:D:251:TYR:HE1	1.05	1.26
1:G:207:HIS:CE1	1:G:251:TYR:HE1	1.55	1.25
1:G:207:HIS:NE2	1:G:251:TYR:HE1	1.05	1.21
1:K:207:HIS:CE1	1:K:251:TYR:HE1	1.62	1.16
1:D:207:HIS:CE1	1:D:251:TYR:HE1	1.63	1.15
1:A:207:HIS:NE2	1:A:251:TYR:HE1	1.14	1.13
1:G:207:HIS:NE2	1:G:251:TYR:CD1	2.18	1.12
3:M:43:ALA:HA	3:M:48:GLU:HB3	1.34	1.09
1:A:207:HIS:CE1	1:A:251:TYR:HE1	1.70	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:HIS:NE2	1:A:251:TYR:CD1	2.21	1.07
1:D:207:HIS:NE2	1:D:251:TYR:CD1	2.23	1.06
1:D:234:VAL:HB	3:F:49:GLU:HG2	1.37	1.05
1:K:207:HIS:NE2	1:K:251:TYR:CD1	2.23	1.04
1:A:207:HIS:CE1	1:A:251:TYR:CE1	2.45	1.03
1:D:462:ALA:HB1	1:D:464:PRO:HD2	1.37	1.03
1:D:418:THR:OG1	3:F:137:ARG:NH1	1.91	1.02
3:M:186:MET:HG2	10:M:402:HEC:ND	1.75	1.01
3:F:37:ASP:HB3	3:F:38:GLN:HA	1.43	1.00
1:G:237:TYR:OH	2:H:8:GLU:OE2	1.81	0.98
3:F:6:SER:OG	3:F:81:ASN:N	1.97	0.97
1:G:207:HIS:CE1	1:G:251:TYR:CE1	2.40	0.97
3:C:186:MET:HG2	10:C:401:HEC:ND	1.78	0.97
3:I:186:MET:HG2	10:I:402:HEC:ND	1.79	0.96
3:F:6:SER:HB2	3:F:81:ASN:HD22	1.28	0.95
1:D:207:HIS:CE1	1:D:251:TYR:CE1	2.45	0.94
3:I:137:ARG:O	3:I:141:ASN:ND2	2.01	0.94
1:K:207:HIS:CE1	1:K:251:TYR:CE1	2.46	0.93
1:G:90:PHE:HD1	1:G:147:GLY:HA3	1.34	0.93
1:D:90:PHE:CD1	1:D:147:GLY:HA3	2.03	0.92
3:F:186:MET:HG2	10:F:401:HEC:ND	1.85	0.92
3:M:68:PHE:HA	3:M:71:LEU:HD12	1.49	0.91
3:M:137:ARG:O	3:M:141:ASN:ND2	2.05	0.90
1:D:24:TRP:HE1	1:D:103:GLN:HE22	1.19	0.90
3:M:36:THR:HG22	3:M:38:GLN:NE2	1.86	0.90
1:K:242:VAL:HG22	3:M:27:THR:HG21	1.54	0.89
3:I:82:TRP:CZ2	3:I:85:VAL:HG23	2.05	0.89
3:C:189:TRP:HZ2	10:C:401:HEC:HMC2	1.35	0.89
1:G:7:THR:O	1:G:469:ALA:HB1	1.71	0.89
3:C:137:ARG:O	3:C:141:ASN:ND2	2.06	0.88
3:F:86:LEU:HG	3:F:87:PRO:HD2	1.57	0.87
1:D:233:PRO:HG2	3:F:50:TYR:CE2	2.09	0.87
1:D:446:ALA:HA	1:D:449:LEU:HD12	1.55	0.87
1:D:156:HIS:CG	3:F:42:HIS:HD2	1.92	0.86
3:F:50:TYR:HB3	3:F:52:ASN:ND2	1.90	0.86
1:A:90:PHE:HD1	1:A:147:GLY:HA3	1.41	0.86
1:G:24:TRP:HE1	1:G:103:GLN:HE22	1.23	0.85
1:G:233:PRO:HG2	3:I:50:TYR:CE2	2.11	0.85
1:A:24:TRP:HE1	1:A:103:GLN:HE22	1.24	0.85
3:F:92:GLY:O	3:F:97:LYS:NZ	2.10	0.85
2:L:7:LEU:HA	2:L:10:ASN:HD22	1.42	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:6:SER:OG	3:M:81:ASN:N	2.08	0.84
3:C:193:ILE:HD11	3:C:228:VAL:HG11	1.59	0.84
3:F:12:LEU:O	3:F:16:THR:OG1	1.95	0.84
3:I:193:ILE:HD11	3:I:228:VAL:HG11	1.58	0.83
1:K:24:TRP:HE1	1:K:103:GLN:HE22	1.22	0.83
9:K:506:PO4:O1	3:M:72:TYR:OH	1.94	0.83
1:G:15:ARG:NH2	1:G:466:GLU:OE2	2.12	0.83
1:A:233:PRO:HG2	3:C:50:TYR:CE2	2.13	0.83
1:D:245:TRP:HZ2	2:E:7:LEU:HD11	1.44	0.83
3:I:6:SER:OG	3:I:81:ASN:N	2.12	0.82
1:A:455:THR:O	1:A:459:VAL:HG23	1.80	0.82
3:I:73:LEU:HB3	3:I:79:LEU:HD11	1.63	0.81
1:K:234:VAL:HB	3:M:49:GLU:HB3	1.62	0.81
3:F:193:ILE:HD11	3:F:228:VAL:HG11	1.61	0.81
1:A:90:PHE:CD1	1:A:147:GLY:HA3	2.15	0.80
3:C:189:TRP:CZ2	10:C:401:HEC:HMC2	2.17	0.80
3:I:207:LYS:HD3	3:I:222:LEU:HD21	1.63	0.80
2:H:68:CYS:HB3	2:H:105:THR:HB	1.61	0.80
1:K:232:ARG:NH1	1:K:295:SER:O	2.14	0.79
3:M:193:ILE:HD11	3:M:228:VAL:HG11	1.63	0.79
1:D:156:HIS:CD2	3:F:42:HIS:HD2	2.01	0.79
2:B:68:CYS:HB3	2:B:105:THR:HB	1.63	0.78
1:G:8:ALA:HA	1:G:469:ALA:HA	1.65	0.78
9:G:506:PO4:O4	3:I:72:TYR:OH	2.00	0.78
2:H:57:ARG:NH2	2:H:97:PRO:O	2.17	0.78
3:I:82:TRP:HZ2	3:I:85:VAL:HG23	1.45	0.78
1:A:335:LEU:HB2	4:N:6:VAL:HG12	1.66	0.78
3:M:24:ILE:HD11	3:M:59:PHE:CZ	2.18	0.78
1:D:267:TRP:HA	3:F:78:GLY:HA2	1.65	0.78
1:D:90:PHE:HD1	1:D:147:GLY:HA3	1.47	0.78
3:I:86:LEU:HD12	3:I:87:PRO:HD2	1.66	0.78
3:I:90:GLU:O	3:I:97:LYS:NZ	2.16	0.78
3:F:90:GLU:O	3:F:97:LYS:NZ	2.16	0.77
1:D:207:HIS:CD2	1:D:251:TYR:CE1	2.71	0.77
3:I:1:MET:HB3	3:I:81:ASN:HD21	1.49	0.77
1:A:207:HIS:CD2	1:A:251:TYR:CE1	2.70	0.77
5:D:502:HEM:HHC	5:D:502:HEM:HBB2	1.67	0.77
1:D:455:THR:O	1:D:459:VAL:HG23	1.86	0.76
5:K:502:HEM:HBC2	5:K:502:HEM:HHD	1.64	0.76
1:G:10:SER:H	1:G:82:GLN:HE22	1.33	0.76
3:M:167:TRP:CE2	3:M:182:ARG:HG2	2.20	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:68:CYS:HB3	2:E:105:THR:HB	1.66	0.76
3:I:6:SER:HB2	3:I:81:ASN:HD22	1.51	0.76
5:D:502:HEM:HBC2	5:D:502:HEM:HHD	1.68	0.76
3:C:6:SER:OG	3:C:81:ASN:N	2.19	0.76
3:I:167:TRP:CE2	3:I:182:ARG:HG2	2.21	0.76
2:L:57:ARG:NH2	2:L:97:PRO:O	2.19	0.75
3:F:40:MET:HB2	3:F:49:GLU:O	1.85	0.75
3:F:60:LEU:HA	3:F:63:ILE:HD11	1.68	0.75
1:K:335:LEU:HB2	4:Q:6:VAL:HG12	1.69	0.75
3:M:86:LEU:HD12	3:M:87:PRO:HD2	1.67	0.75
3:M:242:GLU:OE1	3:M:242:GLU:N	2.18	0.75
3:C:186:MET:HG2	10:C:401:HEC:C4D	2.17	0.74
3:M:2:SER:HG	3:M:5:TRP:HD1	1.34	0.74
1:D:376:HIS:N	1:D:458:THR:HG22	2.03	0.74
5:G:502:HEM:HHC	5:G:502:HEM:HBB2	1.68	0.74
3:M:43:ALA:HA	3:M:48:GLU:CB	2.16	0.74
3:I:195:GLU:OE2	3:I:272:ARG:NH1	2.20	0.74
1:D:335:LEU:HB2	4:O:6:VAL:HG12	1.70	0.74
3:F:73:LEU:HB3	3:F:79:LEU:HD11	1.70	0.74
2:L:177:ASP:N	2:L:177:ASP:OD1	2.21	0.74
1:G:335:LEU:HB2	4:P:6:VAL:HG12	1.70	0.74
3:F:189:TRP:HZ2	10:F:401:HEC:HMC2	1.51	0.73
3:F:189:TRP:CZ2	10:F:401:HEC:HMC2	2.24	0.73
2:B:57:ARG:NH2	2:B:97:PRO:O	2.21	0.73
1:D:416:ASP:OD1	3:F:137:ARG:NH2	2.19	0.73
1:K:242:VAL:CG2	3:M:27:THR:HG21	2.18	0.73
3:I:82:TRP:CZ3	3:I:84:GLY:HA2	2.23	0.73
4:O:23:GLY:O	4:O:27:PHE:HB2	1.89	0.73
5:A:502:HEM:HHC	5:A:502:HEM:HBB2	1.69	0.73
3:F:66:LEU:HD12	3:F:66:LEU:H	1.52	0.73
3:M:44:PHE:N	3:M:47:ILE:O	2.21	0.73
1:A:178:ASN:HD22	1:A:201:VAL:HG12	1.54	0.72
1:G:455:THR:O	1:G:459:VAL:HG23	1.89	0.72
3:M:73:LEU:HD21	3:M:79:LEU:HD21	1.70	0.72
3:M:99:TRP:O	3:M:103:VAL:HG23	1.89	0.72
1:G:115:LEU:HB3	1:G:117:PHE:CE2	2.24	0.72
3:F:167:TRP:CE2	3:F:182:ARG:HG2	2.25	0.72
3:I:36:THR:HG22	3:I:38:GLN:HB2	1.72	0.72
1:A:85:CYS:HB2	1:A:152:ARG:HB2	1.70	0.72
3:C:23:LEU:O	3:C:27:THR:OG1	2.06	0.72
9:D:505:PO4:O3	3:F:72:TYR:OH	2.06	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:1:MET:HB3	3:I:81:ASN:ND2	2.05	0.72
1:G:207:HIS:CD2	1:G:251:TYR:CE1	2.75	0.71
1:A:227:PRO:HB2	3:C:47:ILE:HD12	1.73	0.71
3:F:21:PHE:CE2	3:F:66:LEU:HD22	2.25	0.71
3:M:186:MET:HG2	10:M:402:HEC:C4D	2.20	0.71
3:C:29:LYS:HG3	3:C:30:GLY:N	2.04	0.71
1:K:85:CYS:HB2	1:K:152:ARG:HB2	1.72	0.71
3:C:66:LEU:O	3:C:70:ILE:HD12	1.89	0.71
3:F:6:SER:HB2	3:F:81:ASN:ND2	2.04	0.71
1:D:234:VAL:HB	3:F:49:GLU:CG	2.18	0.71
3:I:189:TRP:HZ2	10:I:402:HEC:HMC2	1.54	0.71
3:C:86:LEU:HD12	3:C:87:PRO:HD2	1.72	0.71
1:K:457:ARG:HH11	1:K:460:GLN:HE21	1.38	0.71
5:K:502:HEM:HHC	5:K:502:HEM:HBB2	1.71	0.71
1:D:10:SER:H	1:D:82:GLN:HE22	1.39	0.70
2:E:57:ARG:NH2	2:E:97:PRO:O	2.24	0.70
5:G:502:HEM:HBC2	5:G:502:HEM:HHD	1.71	0.70
5:A:502:HEM:HBC2	5:A:502:HEM:HHD	1.71	0.70
3:C:195:GLU:OE2	3:C:272:ARG:NH1	2.23	0.70
1:D:85:CYS:HB2	1:D:152:ARG:HB2	1.72	0.70
1:K:207:HIS:CD2	1:K:251:TYR:CE1	2.73	0.70
9:A:506:PO4:O3	3:C:72:TYR:OH	2.06	0.70
3:F:50:TYR:HB3	3:F:52:ASN:HD21	1.57	0.70
1:G:238:ARG:NH2	3:I:30:GLY:O	2.24	0.70
3:I:82:TRP:CH2	3:I:84:GLY:HA2	2.26	0.70
2:B:7:LEU:HA	2:B:10:ASN:HD22	1.54	0.70
1:K:149:LEU:HD21	1:K:161:ASN:HD22	1.57	0.70
1:G:166:ALA:O	1:G:170:THR:HG22	1.92	0.70
4:P:14:VAL:O	4:P:18:VAL:HG23	1.90	0.70
1:A:76:THR:HG21	1:A:221:ILE:HG12	1.72	0.70
3:F:60:LEU:HD23	3:F:63:ILE:HD11	1.73	0.70
1:G:76:THR:HG21	1:G:221:ILE:HG12	1.72	0.70
1:K:235:TYR:HE2	1:K:292:MET:HB3	1.56	0.70
3:C:82:TRP:CH2	3:C:85:VAL:HG23	2.27	0.69
1:D:416:ASP:CG	3:F:137:ARG:HH22	1.95	0.69
1:G:85:CYS:HB2	1:G:152:ARG:HB2	1.74	0.69
2:H:7:LEU:HA	2:H:10:ASN:HD22	1.57	0.69
2:L:68:CYS:HB3	2:L:105:THR:HB	1.73	0.69
1:K:267:TRP:HA	3:M:78:GLY:HA2	1.74	0.69
1:D:156:HIS:CG	3:F:42:HIS:CD2	2.78	0.69
1:K:10:SER:HB3	1:K:89:LEU:CD1	2.21	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:28:ARG:HE	3:M:31:GLU:HG2	1.57	0.69
3:M:43:ALA:CA	3:M:48:GLU:HB3	2.18	0.69
3:M:24:ILE:HD11	3:M:59:PHE:CE2	2.25	0.69
3:M:195:GLU:OE2	3:M:272:ARG:NH1	2.25	0.69
3:I:66:LEU:O	3:I:70:ILE:HD12	1.92	0.69
3:C:167:TRP:CE2	3:C:182:ARG:HG2	2.27	0.69
1:K:467:TYR:O	1:K:468:ASP:HB2	1.93	0.69
1:K:267:TRP:HE1	2:L:36:GLN:HE22	1.41	0.69
1:A:166:ALA:O	1:A:170:THR:HG22	1.93	0.69
1:D:237:TYR:HD1	3:F:49:GLU:OE1	1.76	0.69
1:K:235:TYR:CE2	1:K:292:MET:HB3	2.28	0.69
3:I:76:TYR:C	3:I:82:TRP:HZ3	1.96	0.68
3:F:62:PHE:CD1	3:F:66:LEU:HD11	2.28	0.68
3:M:79:LEU:H	3:M:79:LEU:HD12	1.58	0.68
1:A:31:LEU:HD11	1:A:59:LEU:HD13	1.74	0.68
5:A:501:HEM:HBC2	5:A:501:HEM:HHD	1.75	0.68
2:E:24:ILE:HG21	3:F:16:THR:HG21	1.74	0.68
3:I:189:TRP:CZ2	10:I:402:HEC:HMC2	2.29	0.68
3:I:242:GLU:N	3:I:242:GLU:OE1	2.24	0.68
3:F:74:VAL:HA	3:F:82:TRP:CZ2	2.28	0.68
3:F:186:MET:HG2	10:F:401:HEC:C4D	2.24	0.68
1:K:76:THR:HG21	1:K:221:ILE:HG12	1.76	0.68
1:G:90:PHE:CD1	1:G:147:GLY:HA3	2.24	0.68
1:G:31:LEU:HD11	1:G:59:LEU:HD13	1.76	0.68
1:K:222:MET:HG3	1:K:314:LEU:HD21	1.76	0.68
1:G:376:HIS:N	1:G:458:THR:HG22	2.09	0.67
1:K:463:LYS:CB	1:K:464:PRO:HD3	2.24	0.67
1:G:237:TYR:CE2	1:G:241:ILE:HD11	2.29	0.67
3:F:121:SER:O	3:F:125:VAL:HG23	1.94	0.67
3:F:40:MET:SD	3:F:41:GLY:N	2.68	0.67
1:D:76:THR:HG23	1:D:225:PHE:HE1	1.60	0.67
3:F:121:SER:O	3:F:125:VAL:N	2.28	0.67
3:C:62:PHE:O	3:C:66:LEU:HD12	1.94	0.67
3:F:9:ILE:O	3:F:13:THR:HG23	1.94	0.67
3:I:50:TYR:HB3	3:I:52:ASN:OD1	1.95	0.66
3:I:186:MET:HG2	10:I:402:HEC:C4D	2.24	0.66
1:K:90:PHE:HD2	1:K:91:ALA:N	1.94	0.66
1:D:166:ALA:O	1:D:170:THR:HG22	1.96	0.66
2:L:157:MET:HE1	2:L:171:ASP:HB3	1.77	0.66
1:A:207:HIS:CD2	1:A:251:TYR:CD1	2.83	0.66
3:F:13:THR:O	3:F:17:ILE:HG13	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:61:LEU:O	3:M:65:THR:HG23	1.96	0.66
4:Q:24:PHE:HA	4:Q:27:PHE:HB3	1.78	0.66
3:F:62:PHE:HD1	3:F:66:LEU:HD11	1.61	0.66
2:E:86:TYR:OH	3:F:96:GLU:OE1	2.10	0.66
3:F:99:TRP:O	3:F:103:VAL:HG23	1.96	0.65
1:G:463:LYS:HB2	1:G:464:PRO:HD3	1.76	0.65
3:M:6:SER:HA	3:M:80:GLY:HA2	1.78	0.65
1:A:207:HIS:CD2	1:A:251:TYR:HE1	2.07	0.65
3:C:215:PRO:HB3	11:M:401:FC6:N24	2.12	0.65
1:G:149:LEU:HD21	1:G:161:ASN:HD22	1.62	0.65
1:D:149:LEU:HD21	1:D:161:ASN:HD22	1.61	0.65
1:D:207:HIS:CD2	1:D:251:TYR:CD1	2.85	0.65
1:D:416:ASP:OD1	3:F:137:ARG:NH1	2.30	0.65
3:F:36:THR:O	3:F:38:GLN:NE2	2.30	0.65
1:G:238:ARG:HH12	3:I:30:GLY:C	2.00	0.65
1:A:10:SER:H	1:A:82:GLN:HE22	1.44	0.65
1:A:421:TYR:O	2:B:82:ARG:NH2	2.30	0.65
1:K:421:TYR:O	2:L:82:ARG:NH2	2.30	0.65
2:B:140:TYR:CZ	10:B:301:HEC:HBB2	2.30	0.65
1:D:376:HIS:H	1:D:458:THR:CG2	2.10	0.65
1:K:237:TYR:CE2	1:K:241:ILE:HD11	2.32	0.65
1:K:463:LYS:HB2	1:K:464:PRO:HD3	1.79	0.65
3:M:189:TRP:HZ2	10:M:402:HEC:HMC2	1.62	0.65
1:K:84:THR:HA	3:M:45:ASP:HB2	1.78	0.65
2:E:8:GLU:OE2	3:F:42:HIS:NE2	2.31	0.64
2:H:7:LEU:HD13	2:H:13:LEU:HD22	1.77	0.64
2:H:177:ASP:N	2:H:177:ASP:OD1	2.30	0.64
3:M:117:TYR:CE1	3:M:131:ALA:HB2	2.32	0.64
1:G:267:TRP:HE1	2:H:36:GLN:HE22	1.45	0.64
2:H:86:TYR:OH	3:I:96:GLU:OE1	2.06	0.64
1:K:465:ALA:O	1:K:467:TYR:N	2.30	0.64
2:E:62:ARG:NH1	2:E:63:GLU:OE2	2.28	0.64
4:N:23:GLY:O	4:N:27:PHE:HB2	1.97	0.64
2:E:128:PRO:HD2	2:E:129:ARG:HH21	1.61	0.64
4:O:4:ASP:H	4:O:7:VAL:HG22	1.62	0.64
1:D:355:ALA:O	1:D:359:ILE:HG12	1.97	0.64
3:M:177:SER:OG	3:M:182:ARG:NH1	2.30	0.64
3:M:62:PHE:CD1	3:M:66:LEU:HD11	2.33	0.64
1:A:170:THR:HG21	1:A:212:PHE:CD2	2.33	0.63
3:C:1:MET:HB3	3:C:81:ASN:OD1	1.98	0.63
3:M:189:TRP:CZ2	10:M:402:HEC:HMC2	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:274:VAL:HG21	3:I:73:LEU:CD2	2.27	0.63
1:K:10:SER:HB3	1:K:89:LEU:HD12	1.79	0.63
1:K:233:PRO:HG2	3:M:50:TYR:CZ	2.34	0.63
3:C:25:PHE:HE1	3:C:59:PHE:HZ	1.46	0.63
1:D:376:HIS:H	1:D:458:THR:HG22	1.61	0.63
1:G:336:SER:O	1:G:339:THR:OG1	2.12	0.63
1:G:376:HIS:H	1:G:458:THR:HG22	1.63	0.63
4:Q:14:VAL:O	4:Q:18:VAL:HG23	1.99	0.63
1:K:166:ALA:O	1:K:170:THR:HG22	1.99	0.63
1:G:178:ASN:HD22	1:G:201:VAL:HG12	1.64	0.63
1:G:207:HIS:CD2	1:G:251:TYR:CD1	2.86	0.63
1:G:242:VAL:HG21	3:I:54:LEU:HD21	1.80	0.63
3:M:63:ILE:HA	3:M:66:LEU:HD12	1.80	0.63
1:A:222:MET:HG3	1:A:314:LEU:HD21	1.80	0.63
1:A:340:ASP:H	1:A:406:GLN:HE22	1.47	0.63
1:K:235:TYR:HE2	1:K:292:MET:CB	2.12	0.63
3:C:109:LYS:HG2	3:C:110:TYR:CD2	2.33	0.62
1:D:421:TYR:O	2:E:82:ARG:NH2	2.32	0.62
3:F:128:ASP:OD2	3:F:130:GLN:N	2.31	0.62
1:K:90:PHE:CD1	1:K:147:GLY:HA3	2.34	0.62
1:K:207:HIS:CD2	1:K:251:TYR:CD1	2.87	0.62
1:K:343:ILE:HG12	5:K:502:HEM:HBA2	1.80	0.62
3:M:1:MET:HB3	3:M:81:ASN:OD1	1.99	0.62
1:D:76:THR:HG21	1:D:221:ILE:HG12	1.80	0.62
3:M:94:THR:OG1	3:M:97:LYS:HG3	1.99	0.62
2:E:177:ASP:N	2:E:177:ASP:OD1	2.31	0.62
2:H:157:MET:HE1	2:H:171:ASP:HB3	1.80	0.62
3:M:133:LYS:HE3	3:M:137:ARG:HH21	1.64	0.62
1:A:149:LEU:HD21	1:A:161:ASN:HD22	1.65	0.62
2:B:157:MET:HE1	2:B:171:ASP:HB3	1.81	0.62
1:A:76:THR:HG23	1:A:225:PHE:HE1	1.64	0.62
3:F:29:LYS:CD	3:F:30:GLY:H	2.13	0.62
1:G:170:THR:HG21	1:G:212:PHE:CD2	2.35	0.62
1:K:235:TYR:CE2	1:K:292:MET:CB	2.82	0.62
1:K:455:THR:O	1:K:459:VAL:HG23	2.00	0.62
1:D:178:ASN:HD22	1:D:201:VAL:HG12	1.65	0.62
3:M:28:ARG:HA	3:M:31:GLU:OE2	1.99	0.62
3:M:62:PHE:HE1	3:M:66:LEU:HD21	1.65	0.62
2:B:116:TYR:HE2	3:C:145:ILE:HG21	1.64	0.62
1:G:253:TRP:CH2	2:H:28:THR:HG21	2.34	0.62
1:K:31:LEU:HD11	1:K:59:LEU:HD13	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:TRP:HE1	2:B:36:GLN:HE22	1.48	0.61
4:O:14:VAL:O	4:O:18:VAL:HG23	2.00	0.61
3:F:62:PHE:O	3:F:66:LEU:HD12	2.01	0.61
5:G:501:HEM:HHD	5:G:501:HEM:HBC2	1.82	0.61
1:A:281:ALA:HB3	1:A:282:PRO:HD3	1.81	0.61
2:E:140:TYR:CZ	10:E:301:HEC:HBB2	2.34	0.61
3:F:29:LYS:HD2	3:F:30:GLY:H	1.64	0.61
1:G:236:SER:HA	3:I:52:ASN:HB2	1.82	0.61
3:C:109:LYS:HG2	3:C:110:TYR:CE2	2.34	0.61
1:A:63:ALA:O	1:A:67:ALA:HB3	2.01	0.61
1:A:218:PHE:HA	1:A:221:ILE:HG13	1.82	0.61
3:C:99:TRP:O	3:C:103:VAL:HG23	2.00	0.61
1:D:343:ILE:HG12	5:D:502:HEM:HBA2	1.83	0.61
4:Q:24:PHE:O	4:Q:28:ILE:HG13	2.01	0.61
2:B:177:ASP:OD1	2:B:177:ASP:N	2.33	0.60
3:F:83:LYS:NZ	3:F:91:GLY:O	2.17	0.60
2:H:39:VAL:HG23	2:H:40:ASN:ND2	2.16	0.60
1:A:237:TYR:CE2	1:A:241:ILE:HD11	2.35	0.60
3:I:39:THR:HG22	3:I:40:MET:O	2.01	0.60
2:H:140:TYR:CZ	10:H:301:HEC:HBB2	2.35	0.60
3:I:97:LYS:O	3:I:101:ARG:HG3	2.01	0.60
2:B:62:ARG:NH1	2:B:63:GLU:OE2	2.31	0.60
1:A:228:LYS:NZ	3:C:45:ASP:OD1	2.31	0.60
3:I:24:ILE:HD12	3:I:59:PHE:HE2	1.66	0.60
3:I:36:THR:CG2	3:I:38:GLN:HB2	2.31	0.60
11:C:403:FC6:N24	3:M:215:PRO:HB3	2.17	0.60
3:F:195:GLU:OE2	3:F:272:ARG:NH1	2.35	0.60
1:K:76:THR:HG23	1:K:225:PHE:HE1	1.66	0.60
1:D:63:ALA:O	1:D:67:ALA:HB3	2.01	0.60
3:F:187:PRO:HG2	3:F:189:TRP:CZ2	2.37	0.60
1:K:178:ASN:HD22	1:K:201:VAL:HG12	1.67	0.60
3:C:271:ILE:HG12	10:C:401:HEC:HMB2	1.84	0.60
3:C:61:LEU:O	3:C:65:THR:HG23	2.02	0.60
1:G:63:ALA:O	1:G:67:ALA:HB3	2.01	0.60
1:K:235:TYR:CD1	1:K:236:SER:N	2.70	0.60
1:A:291:MET:SD	4:N:24:PHE:CZ	2.95	0.60
1:D:252:ILE:HD11	2:E:22:VAL:HG22	1.84	0.60
3:F:74:VAL:HA	3:F:82:TRP:HZ2	1.67	0.60
1:G:281:ALA:HB3	1:G:282:PRO:HD3	1.84	0.60
1:G:468:ASP:OD1	1:G:470:ALA:N	2.35	0.60
3:I:178:ILE:HG12	10:I:403:HEC:HMB2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:319:MET:HB2	4:Q:21:LEU:HD21	1.84	0.60
3:C:59:PHE:CE1	3:C:63:ILE:HD11	2.37	0.59
1:D:417:GLY:N	3:F:110:TYR:CE2	2.70	0.59
1:A:346:VAL:HG22	5:A:501:HEM:C2D	2.37	0.59
3:I:86:LEU:HD12	3:I:87:PRO:CD	2.31	0.59
1:D:238:ARG:HH12	3:F:30:GLY:C	2.05	0.59
1:D:31:LEU:HD11	1:D:59:LEU:HD13	1.85	0.59
3:C:62:PHE:CD1	3:C:66:LEU:HD11	2.38	0.59
1:G:227:PRO:HB2	3:I:47:ILE:HD12	1.82	0.59
11:F:403:FC6:N24	3:I:215:PRO:HB3	2.17	0.59
2:L:140:TYR:CZ	10:L:301:HEC:HBB2	2.38	0.59
3:I:4:PHE:CD1	3:I:4:PHE:C	2.75	0.59
1:A:370:PHE:CE2	1:A:459:VAL:HG13	2.37	0.59
1:G:343:ILE:HG12	5:G:502:HEM:HBA2	1.85	0.59
3:I:89:TYR:CD1	3:I:93:TRP:CD1	2.91	0.59
2:B:193:GLN:HA	2:B:193:GLN:HE21	1.66	0.59
3:F:89:TYR:C	3:F:97:LYS:HZ3	2.05	0.59
3:I:127:GLN:HA	3:I:127:GLN:HE21	1.68	0.59
1:K:230:ALA:O	1:K:300:LYS:NZ	2.33	0.59
3:C:93:TRP:HE1	3:C:98:GLN:HE21	1.51	0.58
3:I:99:TRP:O	3:I:103:VAL:HG23	2.03	0.58
2:L:62:ARG:NH1	2:L:63:GLU:OE2	2.35	0.58
3:F:60:LEU:O	3:F:63:ILE:HG12	2.02	0.58
3:I:63:ILE:O	3:I:67:VAL:HG23	2.02	0.58
3:F:271:ILE:HG12	10:F:401:HEC:HMB2	1.85	0.58
1:A:17:PHE:CZ	1:A:99:PHE:HA	2.39	0.58
1:K:457:ARG:HH11	1:K:460:GLN:NE2	2.01	0.58
5:K:501:HEM:HBC2	5:K:501:HEM:HHD	1.83	0.58
3:M:24:ILE:CG1	3:M:59:PHE:HE2	2.16	0.58
1:K:63:ALA:O	1:K:67:ALA:HB3	2.04	0.58
1:K:10:SER:N	1:K:82:GLN:HE22	2.02	0.58
3:C:29:LYS:HG3	3:C:30:GLY:H	1.66	0.58
3:F:82:TRP:C	3:F:82:TRP:CD1	2.77	0.58
1:G:347:HIS:HA	1:G:350:ALA:HB3	1.84	0.58
3:I:137:ARG:HH11	3:I:137:ARG:HG2	1.68	0.58
3:M:207:LYS:HD3	3:M:222:LEU:HD21	1.86	0.58
1:D:218:PHE:HA	1:D:221:ILE:HG13	1.85	0.58
1:D:253:TRP:CZ3	3:F:13:THR:HG22	2.39	0.58
3:C:178:ILE:HG12	10:C:402:HEC:HMB2	1.86	0.58
3:F:40:MET:N	3:F:49:GLU:O	2.37	0.58
1:D:253:TRP:CH2	2:E:28:THR:HG21	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:222:MET:HG3	1:G:314:LEU:HD21	1.85	0.57
1:G:218:PHE:HA	1:G:221:ILE:HG13	1.87	0.57
3:M:63:ILE:O	3:M:67:VAL:HG23	2.04	0.57
1:A:13:VAL:HA	1:A:16:GLN:HE21	1.70	0.57
1:K:235:TYR:HD1	1:K:236:SER:N	2.03	0.57
1:G:10:SER:N	1:G:82:GLN:HE22	2.02	0.57
1:D:359:ILE:HD12	1:D:451:MET:HE3	1.85	0.57
3:I:117:TYR:CZ	3:I:131:ALA:HB2	2.40	0.57
3:C:128:ASP:OD2	3:C:131:ALA:N	2.32	0.57
1:D:57:ARG:NH2	5:D:502:HEM:O2D	2.37	0.57
3:M:110:TYR:HA	3:M:113:ILE:HG13	1.86	0.57
3:M:24:ILE:HD11	3:M:59:PHE:HZ	1.66	0.57
3:I:74:VAL:O	3:I:82:TRP:CZ2	2.58	0.57
1:K:347:HIS:HA	1:K:350:ALA:HB3	1.85	0.57
3:C:25:PHE:CE1	3:C:59:PHE:HZ	2.23	0.57
1:D:242:VAL:HG22	3:F:27:THR:HG21	1.86	0.57
1:D:410:TRP:O	2:E:82:ARG:NH1	2.37	0.57
4:Q:27:PHE:CD2	4:Q:27:PHE:C	2.78	0.57
1:A:453:TYR:O	1:A:457:ARG:HG2	2.05	0.57
3:F:63:ILE:HA	3:F:66:LEU:CD1	2.34	0.57
1:K:242:VAL:HG21	3:M:54:LEU:HD21	1.87	0.57
4:P:24:PHE:HE1	4:P:28:ILE:HD11	1.69	0.57
3:C:89:TYR:CE1	3:C:93:TRP:CD1	2.93	0.56
3:F:79:LEU:O	3:F:82:TRP:HB3	2.04	0.56
1:K:218:PHE:HA	1:K:221:ILE:HG13	1.85	0.56
1:G:342:THR:O	1:G:346:VAL:HG23	2.05	0.56
3:F:35:THR:O	3:F:52:ASN:OD1	2.24	0.56
5:D:501:HEM:HBC2	5:D:501:HEM:HHD	1.87	0.56
3:I:4:PHE:HD1	3:I:4:PHE:O	1.87	0.56
3:M:62:PHE:CE1	3:M:66:LEU:HD21	2.40	0.56
1:A:347:HIS:HA	1:A:350:ALA:HB3	1.88	0.56
2:E:6:LYS:HD3	2:E:8:GLU:OE2	2.06	0.56
1:D:233:PRO:HG2	3:F:50:TYR:CZ	2.41	0.56
1:G:115:LEU:HD23	1:G:117:PHE:HE2	1.70	0.56
1:G:291:MET:SD	4:P:24:PHE:HZ	2.28	0.56
1:A:411:ARG:NH1	4:N:4:ASP:OD2	2.39	0.56
1:A:211:GLY:O	1:A:215:THR:HB	2.06	0.56
3:I:140:ALA:O	3:I:144:SER:OG	2.18	0.56
1:K:235:TYR:CE1	1:K:236:SER:HB2	2.41	0.56
1:K:237:TYR:HB2	3:M:49:GLU:HG3	1.87	0.56
2:E:157:MET:HE1	2:E:171:ASP:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:20:LEU:HD22	3:M:62:PHE:HZ	1.70	0.56
1:A:359:ILE:HD11	1:A:448:MET:CE	2.36	0.56
3:C:89:TYR:CD2	3:C:101:ARG:NH1	2.74	0.56
3:F:123:GLU:O	3:F:126:ALA:HB3	2.06	0.56
1:D:281:ALA:HB3	1:D:282:PRO:HD3	1.87	0.56
1:K:170:THR:HG21	1:K:212:PHE:CD2	2.41	0.56
1:A:57:ARG:NH1	5:A:502:HEM:O2A	2.39	0.55
1:A:253:TRP:CH2	2:B:28:THR:HG21	2.40	0.55
1:D:222:MET:HG3	1:D:314:LEU:HD21	1.87	0.55
1:D:245:TRP:CZ2	2:E:7:LEU:HD11	2.32	0.55
3:C:94:THR:OG1	3:C:97:LYS:HG3	2.06	0.55
1:D:347:HIS:HA	1:D:350:ALA:HB3	1.87	0.55
1:K:281:ALA:HB3	1:K:282:PRO:HD3	1.88	0.55
1:D:8:ALA:HA	1:D:469:ALA:O	2.06	0.55
3:I:116:LYS:O	3:I:120:MET:HG3	2.06	0.55
3:I:38:GLN:CD	3:I:39:THR:H	2.09	0.55
3:I:89:TYR:CE1	3:I:93:TRP:CD1	2.95	0.55
3:M:8:TYR:HE2	3:M:12:LEU:HD12	1.71	0.55
1:K:457:ARG:NH1	1:K:460:GLN:NE2	2.55	0.55
3:F:24:ILE:HG13	3:F:59:PHE:HE1	1.71	0.55
1:G:352:GLY:O	1:G:356:MET:HG3	2.06	0.55
3:F:63:ILE:HA	3:F:66:LEU:HD13	1.88	0.55
3:F:83:LYS:HD2	3:F:92:GLY:HA3	1.89	0.55
1:G:421:TYR:O	2:H:82:ARG:NH2	2.40	0.55
1:G:376:HIS:H	1:G:458:THR:CG2	2.19	0.55
1:K:376:HIS:N	1:K:458:THR:HG22	2.22	0.55
1:A:359:ILE:HD11	1:A:448:MET:HE1	1.88	0.55
1:D:211:GLY:O	1:D:215:THR:HB	2.07	0.55
1:D:235:TYR:CE1	1:D:236:SER:HB2	2.42	0.55
1:G:242:VAL:HG22	3:I:27:THR:HG21	1.89	0.55
1:A:233:PRO:CG	3:C:50:TYR:CE2	2.89	0.55
3:C:81:ASN:O	3:C:83:LYS:HD3	2.07	0.55
1:A:252:ILE:HD11	2:B:22:VAL:HG22	1.89	0.54
3:C:63:ILE:O	3:C:67:VAL:HG23	2.07	0.54
2:E:42:PRO:HG3	2:E:93:VAL:HG11	1.89	0.54
3:F:111:GLY:N	3:F:112:PRO:HD2	2.22	0.54
1:G:230:ALA:O	1:G:300:LYS:NZ	2.34	0.54
1:K:264:LEU:HD12	1:K:265:PRO:HD2	1.89	0.54
3:M:105:GLN:HB3	3:M:109:LYS:NZ	2.22	0.54
3:M:28:ARG:O	3:M:31:GLU:HB2	2.07	0.54
1:A:376:HIS:HB2	1:A:458:THR:HG22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:6:LYS:O	2:E:7:LEU:HG	2.06	0.54
1:D:237:TYR:OH	2:E:8:GLU:OE1	2.25	0.54
3:F:177:SER:OG	3:F:182:ARG:NH1	2.36	0.54
3:I:74:VAL:O	3:I:82:TRP:CH2	2.60	0.54
1:K:17:PHE:CZ	1:K:99:PHE:HA	2.42	0.54
2:L:37:ASP:O	2:L:41:GLU:HG3	2.07	0.54
3:C:50:TYR:HD1	3:C:52:ASN:HD21	1.56	0.54
3:I:76:TYR:CE1	3:I:86:LEU:HD22	2.42	0.54
3:M:59:PHE:CE1	3:M:63:ILE:HD11	2.42	0.54
1:D:238:ARG:NH2	3:F:30:GLY:O	2.40	0.54
1:D:352:GLY:O	1:D:356:MET:HG3	2.08	0.54
4:N:14:VAL:O	4:N:18:VAL:HG23	2.07	0.54
3:C:207:LYS:HD3	3:C:222:LEU:HD21	1.89	0.54
2:H:70:SER:HA	2:H:101:GLY:HA3	1.89	0.54
1:K:340:ASP:H	1:K:406:GLN:HE22	1.55	0.54
3:M:37:ASP:C	3:M:38:GLN:NE2	2.61	0.54
1:D:13:VAL:HA	1:D:16:GLN:HE21	1.73	0.54
3:F:63:ILE:O	3:F:67:VAL:HG23	2.06	0.54
1:K:331:THR:OG1	9:K:506:PO4:O2	2.22	0.54
1:K:10:SER:H	1:K:82:GLN:HE22	1.54	0.54
2:L:6:LYS:O	2:L:7:LEU:HG	2.07	0.54
3:M:187:PRO:HG2	3:M:189:TRP:CZ2	2.43	0.54
3:C:206:ARG:NH1	3:C:262:SER:O	2.40	0.54
3:F:97:LYS:HE2	3:F:101:ARG:HH12	1.73	0.54
1:K:13:VAL:HA	1:K:16:GLN:HE21	1.72	0.54
1:K:211:GLY:O	1:K:215:THR:HB	2.08	0.54
3:M:62:PHE:CE1	3:M:66:LEU:HD11	2.43	0.54
1:A:342:THR:O	1:A:346:VAL:HG23	2.07	0.54
1:D:170:THR:HG21	1:D:212:PHE:CD2	2.43	0.54
1:D:233:PRO:HB3	3:F:48:GLU:HG3	1.89	0.54
1:D:234:VAL:O	3:F:50:TYR:N	2.41	0.54
2:H:39:VAL:HG23	2:H:40:ASN:HD22	1.73	0.54
3:M:37:ASP:O	3:M:38:GLN:NE2	2.41	0.54
1:D:267:TRP:HE1	2:E:36:GLN:HE22	1.56	0.54
2:B:128:PRO:HD2	2:B:129:ARG:HH21	1.73	0.54
2:E:70:SER:HA	2:E:101:GLY:HA3	1.90	0.54
3:F:66:LEU:O	3:F:70:ILE:HG12	2.07	0.54
1:G:64:VAL:HG11	5:G:502:HEM:C4C	2.43	0.54
3:M:66:LEU:O	3:M:70:ILE:HG13	2.07	0.54
3:I:177:SER:HA	3:I:182:ARG:HD2	1.91	0.53
3:M:186:MET:HG2	10:M:402:HEC:C1D	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:12:LEU:O	3:C:16:THR:OG1	2.26	0.53
3:F:37:ASP:OD2	3:F:50:TYR:CD1	2.62	0.53
1:D:17:PHE:CZ	1:D:99:PHE:HA	2.43	0.53
1:D:10:SER:N	1:D:82:GLN:HE22	2.04	0.53
1:D:371:GLY:HA3	1:D:467:TYR:CD1	2.43	0.53
1:G:17:PHE:CZ	1:G:99:PHE:HA	2.43	0.53
3:F:76:TYR:CZ	3:F:86:LEU:HD13	2.44	0.53
1:G:370:PHE:CE2	1:G:459:VAL:HG13	2.43	0.53
1:G:76:THR:HG23	1:G:225:PHE:HE1	1.73	0.53
1:D:446:ALA:O	1:D:450:VAL:HG23	2.08	0.53
1:A:352:GLY:O	1:A:356:MET:HG3	2.08	0.53
1:D:340:ASP:H	1:D:406:GLN:HE22	1.55	0.53
3:F:60:LEU:HA	3:F:63:ILE:CD1	2.37	0.53
3:I:167:TRP:CD2	3:I:182:ARG:HG2	2.44	0.53
3:M:24:ILE:HD13	3:M:24:ILE:C	2.28	0.53
1:A:239:LEU:HD23	1:A:289:ASN:HD22	1.74	0.53
2:H:193:GLN:HA	2:H:193:GLN:HE21	1.74	0.53
1:D:340:ASP:H	1:D:406:GLN:NE2	2.07	0.53
2:E:86:TYR:HE2	3:F:99:TRP:CE3	2.27	0.53
3:F:120:MET:CE	3:F:124:GLU:HB3	2.39	0.53
3:M:39:THR:HG22	3:M:40:MET:O	2.09	0.53
1:G:82:GLN:NE2	1:G:89:LEU:H	2.07	0.53
2:L:128:PRO:HD2	2:L:129:ARG:HH21	1.74	0.53
1:G:291:MET:SD	4:P:24:PHE:CZ	3.02	0.52
1:A:340:ASP:H	1:A:406:GLN:NE2	2.07	0.52
1:D:261:TYR:HA	3:F:95:GLN:OE1	2.09	0.52
3:F:8:TYR:O	3:F:12:LEU:HD12	2.09	0.52
1:G:152:ARG:NH2	2:H:9:LYS:O	2.42	0.52
3:I:61:LEU:O	3:I:65:THR:HG23	2.08	0.52
1:K:253:TRP:CH2	2:L:28:THR:HG21	2.44	0.52
1:G:239:LEU:HD23	1:G:289:ASN:HD22	1.74	0.52
1:D:10:SER:H	1:D:82:GLN:NE2	2.08	0.52
3:F:45:ASP:CG	3:F:46:GLY:H	2.13	0.52
3:I:8:TYR:O	3:I:12:LEU:HD12	2.10	0.52
1:K:330:LYS:HB2	9:K:506:PO4:O1	2.10	0.52
1:K:82:GLN:CG	1:K:89:LEU:HG	2.39	0.52
2:L:193:GLN:HE21	2:L:193:GLN:HA	1.74	0.52
1:K:238:ARG:NH2	3:M:51:ASP:OD1	2.41	0.52
3:I:177:SER:OG	3:I:182:ARG:NH1	2.40	0.52
1:G:236:SER:CA	3:I:52:ASN:HB2	2.39	0.52
3:M:2:SER:OG	3:M:5:TRP:HD1	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:62:ASN:HD21	1:D:125:GLU:HG3	1.74	0.52
1:G:274:VAL:HG21	3:I:73:LEU:HD21	1.89	0.52
3:M:11:LEU:HD23	3:M:12:LEU:N	2.24	0.52
1:D:346:VAL:HG22	5:D:501:HEM:C2D	2.44	0.52
1:G:267:TRP:HA	3:I:78:GLY:HA2	1.92	0.52
3:I:17:ILE:HG23	3:I:66:LEU:CD2	2.40	0.52
3:M:97:LYS:O	3:M:101:ARG:HG3	2.09	0.52
3:F:114:PHE:HB3	3:F:289:ASP:OD2	2.09	0.52
2:E:24:ILE:HG21	3:F:16:THR:CG2	2.39	0.52
3:F:178:ILE:HG12	10:F:402:HEC:HMB2	1.91	0.52
2:E:152:ASP:HA	2:E:155:LYS:HE3	1.92	0.52
3:F:29:LYS:CD	3:F:30:GLY:N	2.73	0.52
3:F:34:GLY:O	3:F:36:THR:OG1	2.26	0.52
1:K:227:PRO:CB	3:M:47:ILE:HG21	2.39	0.52
1:G:359:ILE:HD11	1:G:448:MET:HE1	1.92	0.51
1:K:321:THR:HG22	5:K:501:HEM:HAB	1.93	0.51
2:H:63:GLU:HB3	10:H:301:HEC:HBB1	1.90	0.51
3:I:25:PHE:HE1	3:I:59:PHE:HZ	1.58	0.51
3:F:40:MET:HB2	3:F:49:GLU:HB2	1.92	0.51
1:K:352:GLY:O	1:K:356:MET:HG3	2.09	0.51
1:A:64:VAL:HG11	5:A:502:HEM:C4C	2.45	0.51
1:D:207:HIS:CD2	1:D:251:TYR:HE1	2.07	0.51
3:M:8:TYR:HE2	3:M:12:LEU:CD1	2.23	0.51
2:B:152:ASP:HA	2:B:155:LYS:HE3	1.92	0.51
1:D:301:LEU:HD21	1:D:311:VAL:HG21	1.93	0.51
2:E:193:GLN:HA	2:E:193:GLN:HE21	1.74	0.51
3:F:75:LEU:HD22	3:F:86:LEU:HD12	1.92	0.51
1:G:395:TYR:CZ	1:G:437:ARG:HD2	2.46	0.51
2:H:128:PRO:HD2	2:H:129:ARG:HH21	1.75	0.51
3:M:116:LYS:O	3:M:120:MET:HG3	2.11	0.51
3:M:73:LEU:HG	3:M:79:LEU:HD11	1.92	0.51
3:C:62:PHE:CE1	3:C:66:LEU:HD11	2.46	0.51
3:F:77:PRO:HG3	3:F:93:TRP:O	2.10	0.51
3:I:117:TYR:CE1	3:I:131:ALA:HB2	2.46	0.51
3:I:56:ARG:O	3:I:59:PHE:HB3	2.09	0.51
1:A:355:ALA:O	1:A:359:ILE:HG12	2.11	0.51
3:C:59:PHE:CZ	3:C:63:ILE:HD11	2.45	0.51
3:F:206:ARG:NH1	3:F:262:SER:O	2.42	0.51
3:I:4:PHE:HD1	3:I:4:PHE:C	2.14	0.51
3:I:73:LEU:HB3	3:I:79:LEU:CD1	2.37	0.51
4:P:24:PHE:CE1	4:P:28:ILE:HD11	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:37:ASP:CB	3:F:38:GLN:HA	2.28	0.51
1:G:10:SER:H	1:G:82:GLN:NE2	2.03	0.51
1:G:252:ILE:HD11	2:H:22:VAL:HG22	1.93	0.51
1:G:355:ALA:O	1:G:359:ILE:HG12	2.11	0.51
1:G:375:MET:CE	1:G:458:THR:HG21	2.41	0.51
2:L:7:LEU:HD12	2:L:7:LEU:O	2.11	0.51
3:M:11:LEU:HD23	3:M:12:LEU:HG	1.93	0.51
2:B:157:MET:HE2	2:B:172:ILE:HA	1.91	0.51
3:I:89:TYR:HA	3:I:101:ARG:NH2	2.26	0.51
3:M:121:SER:O	3:M:125:VAL:HG23	2.10	0.51
3:M:177:SER:HA	3:M:182:ARG:HD2	1.92	0.51
3:M:81:ASN:O	3:M:83:LYS:HD3	2.10	0.51
3:C:74:VAL:O	3:C:82:TRP:CH2	2.64	0.51
1:D:82:GLN:NE2	1:D:89:LEU:H	2.09	0.51
3:F:24:ILE:HG13	3:F:59:PHE:CE1	2.46	0.51
3:F:89:TYR:HD1	3:F:93:TRP:HD1	1.57	0.51
1:K:154:VAL:HG21	3:M:44:PHE:CE2	2.46	0.51
3:M:21:PHE:CE2	3:M:66:LEU:HD13	2.46	0.51
1:A:115:LEU:HB3	1:A:117:PHE:CE2	2.46	0.50
2:B:70:SER:HA	2:B:101:GLY:HA3	1.91	0.50
2:E:140:TYR:CE1	10:E:301:HEC:HBB2	2.46	0.50
3:C:215:PRO:HG3	11:M:401:FC6:N25	2.27	0.50
1:G:235:TYR:CE1	1:G:236:SER:HB2	2.47	0.50
1:K:350:ALA:HB1	5:K:502:HEM:CAC	2.41	0.50
5:K:501:HEM:HBB2	5:K:501:HEM:HMB1	1.92	0.50
2:L:6:LYS:HD3	2:L:8:GLU:OE2	2.11	0.50
3:M:179:LEU:HD22	3:M:283:GLN:HB2	1.94	0.50
3:F:167:TRP:CD2	3:F:182:ARG:HG2	2.46	0.50
1:K:313:SER:HB2	1:K:356:MET:HB2	1.93	0.50
2:B:62:ARG:HG3	2:B:63:GLU:N	2.27	0.50
3:C:50:TYR:CB	3:C:52:ASN:ND2	2.74	0.50
1:D:416:ASP:OD1	3:F:137:ARG:CZ	2.59	0.50
1:K:359:ILE:HD12	1:K:384:HIS:HE1	1.75	0.50
3:C:167:TRP:CD2	3:C:182:ARG:HG2	2.46	0.50
1:K:82:GLN:HE21	1:K:88:THR:HA	1.76	0.50
3:C:28:ARG:O	3:C:28:ARG:HG2	2.12	0.50
1:A:370:PHE:C	1:A:465:ALA:HB1	2.31	0.50
3:M:23:LEU:O	3:M:27:THR:OG1	2.28	0.50
1:A:169:LEU:HD11	2:B:15:THR:HG23	1.94	0.50
1:D:156:HIS:CD2	3:F:42:HIS:CD2	2.92	0.50
2:E:39:VAL:HG23	2:E:40:ASN:ND2	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:211:GLY:O	1:G:215:THR:HB	2.11	0.50
2:H:148:LEU:HD11	2:H:187:ALA:HB2	1.94	0.50
1:K:235:TYR:CE1	3:M:52:ASN:ND2	2.79	0.50
1:A:82:GLN:NE2	1:A:89:LEU:H	2.09	0.50
1:D:239:LEU:HD23	1:D:289:ASN:HD22	1.76	0.50
3:F:131:ALA:O	3:F:134:MET:HB3	2.12	0.50
1:G:156:HIS:CD2	3:I:42:HIS:CD2	3.00	0.50
1:K:169:LEU:HD11	2:L:15:THR:HG23	1.94	0.50
1:K:342:THR:O	1:K:346:VAL:HG23	2.11	0.50
3:M:133:LYS:HE3	3:M:137:ARG:NH2	2.27	0.50
2:B:6:LYS:O	2:B:7:LEU:HG	2.12	0.49
1:A:10:SER:N	1:A:82:GLN:HE22	2.10	0.49
1:A:94:LEU:O	1:A:98:THR:HG23	2.12	0.49
3:M:37:ASP:C	3:M:38:GLN:HE21	2.16	0.49
1:A:238:ARG:NH2	3:C:30:GLY:O	2.45	0.49
3:F:1:MET:HB3	3:F:81:ASN:ND2	2.27	0.49
1:G:120:SER:OG	2:H:97:PRO:HG2	2.13	0.49
3:I:239:GLN:N	3:I:239:GLN:OE1	2.26	0.49
1:K:10:SER:O	1:K:89:LEU:HD11	2.12	0.49
1:K:235:TYR:CD2	1:K:292:MET:HB2	2.47	0.49
1:K:64:VAL:HG11	5:K:502:HEM:C4C	2.47	0.49
1:G:359:ILE:HD12	1:G:384:HIS:HE1	1.77	0.49
1:G:346:VAL:HG22	5:G:501:HEM:C2D	2.47	0.49
3:I:21:PHE:O	3:I:24:ILE:HG22	2.12	0.49
2:L:63:GLU:HB3	10:L:301:HEC:HBB1	1.93	0.49
1:K:238:ARG:HG3	3:M:51:ASP:OD2	2.12	0.49
4:O:2:PHE:CE2	4:O:4:ASP:HB2	2.48	0.49
3:F:29:LYS:HD3	3:F:30:GLY:N	2.27	0.49
3:F:66:LEU:HD12	3:F:66:LEU:N	2.23	0.49
1:K:8:ALA:HA	1:K:469:ALA:HA	1.93	0.49
3:M:28:ARG:NH1	3:M:59:PHE:CE1	2.80	0.49
2:L:86:TYR:HE2	3:M:99:TRP:CE3	2.30	0.49
4:O:4:ASP:H	4:O:7:VAL:CG2	2.25	0.49
3:I:76:TYR:C	3:I:82:TRP:CZ3	2.83	0.49
3:M:122:VAL:HG22	3:M:292:HIS:CD2	2.46	0.49
1:A:15:ARG:HG2	1:A:370:PHE:CZ	2.48	0.49
1:D:455:THR:C	1:D:459:VAL:HG23	2.33	0.49
1:G:238:ARG:O	1:G:242:VAL:HG23	2.12	0.49
3:I:271:ILE:HG12	10:I:402:HEC:HMB2	1.93	0.49
3:M:28:ARG:HG3	3:M:31:GLU:CD	2.32	0.49
3:F:2:SER:HG	3:F:5:TRP:HD1	1.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:6:SER:CB	3:F:81:ASN:HD22	2.14	0.49
1:G:155:LYS:HE3	2:H:9:LYS:NZ	2.27	0.49
2:E:43:VAL:HG13	2:E:46:MET:HB2	1.95	0.49
3:F:229:TYR:HE1	3:F:239:GLN:HA	1.77	0.49
3:F:89:TYR:HD1	3:F:93:TRP:CD1	2.31	0.49
3:M:21:PHE:O	3:M:24:ILE:HG22	2.13	0.49
2:B:43:VAL:HG13	2:B:46:MET:HB2	1.93	0.48
1:D:313:SER:HB2	1:D:356:MET:HB2	1.94	0.48
3:F:6:SER:HG	3:F:81:ASN:H	1.51	0.48
1:G:15:ARG:HG2	1:G:370:PHE:CZ	2.48	0.48
2:H:88:VAL:HG12	2:H:90:GLY:H	1.78	0.48
3:I:89:TYR:CD1	3:I:93:TRP:HD1	2.30	0.48
3:C:114:PHE:CE1	3:C:134:MET:HE1	2.48	0.48
3:C:122:VAL:HG22	3:C:292:HIS:CD2	2.47	0.48
1:D:238:ARG:O	1:D:242:VAL:HG23	2.13	0.48
1:D:416:ASP:C	3:F:110:TYR:CE2	2.86	0.48
3:F:26:ALA:O	3:F:29:LYS:HG3	2.13	0.48
3:F:54:LEU:HD22	3:F:54:LEU:H	1.78	0.48
1:G:468:ASP:OD1	1:G:469:ALA:N	2.45	0.48
1:G:169:LEU:HD11	2:H:15:THR:HG23	1.95	0.48
2:L:70:SER:HA	2:L:101:GLY:HA3	1.93	0.48
3:C:73:LEU:HB3	3:C:79:LEU:HD11	1.94	0.48
1:D:342:THR:O	1:D:346:VAL:HG23	2.12	0.48
1:G:125:GLU:HG2	1:G:125:GLU:H	1.36	0.48
3:M:62:PHE:O	3:M:66:LEU:HG	2.13	0.48
2:B:39:VAL:HG23	2:B:40:ASN:ND2	2.27	0.48
1:A:418:THR:OG1	3:C:137:ARG:HD2	2.13	0.48
3:C:166:ARG:HH21	10:C:401:HEC:HAD2	1.79	0.48
3:F:89:TYR:CD2	3:F:101:ARG:NH1	2.82	0.48
1:G:359:ILE:HD12	1:G:384:HIS:CE1	2.48	0.48
2:H:140:TYR:CE1	10:H:301:HEC:HBB2	2.48	0.48
1:D:84:THR:O	3:F:44:PHE:HD2	1.95	0.48
1:D:233:PRO:CG	3:F:50:TYR:CE2	2.90	0.48
1:G:57:ARG:NH1	5:G:502:HEM:O2A	2.46	0.48
3:M:28:ARG:HG3	3:M:31:GLU:OE2	2.13	0.48
1:A:384:HIS:CE1	1:A:451:MET:HB2	2.49	0.48
3:C:184:ALA:HB1	10:C:401:HEC:HMD1	1.96	0.48
3:F:123:GLU:O	3:F:127:GLN:HG3	2.14	0.48
3:I:179:LEU:HD23	3:I:291:VAL:HG11	1.96	0.48
3:M:37:ASP:OD1	3:M:38:GLN:N	2.46	0.48
1:D:415:ASP:O	3:F:110:TYR:CE2	2.67	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:416:ASP:CA	3:F:110:TYR:HE2	2.26	0.48
1:G:159:VAL:HA	1:G:162:TRP:CD2	2.49	0.48
1:K:340:ASP:H	1:K:406:GLN:NE2	2.12	0.48
1:K:233:PRO:CG	3:M:50:TYR:CZ	2.97	0.48
1:G:384:HIS:CE1	1:G:451:MET:HB2	2.49	0.48
2:L:62:ARG:HH22	2:L:184:GLU:CD	2.17	0.48
2:B:161:ARG:HA	2:B:165:VAL:O	2.14	0.48
1:D:159:VAL:HA	1:D:162:TRP:CD2	2.49	0.48
3:F:179:LEU:HD23	3:F:291:VAL:HG11	1.94	0.48
3:F:40:MET:SD	3:F:42:HIS:ND1	2.87	0.48
3:M:255:ALA:HA	3:M:258:TRP:CD2	2.49	0.48
2:B:63:GLU:HB3	10:B:301:HEC:HBB1	1.96	0.48
1:K:376:HIS:H	1:K:458:THR:CG2	2.27	0.48
1:A:310:LEU:O	1:A:313:SER:HB3	2.13	0.47
3:C:189:TRP:O	3:C:193:ILE:HG22	2.14	0.47
3:M:111:GLY:N	3:M:112:PRO:CD	2.77	0.47
3:M:178:ILE:HG12	10:M:403:HEC:HMB2	1.96	0.47
1:A:416:ASP:OD2	3:C:137:ARG:NH1	2.47	0.47
1:D:76:THR:HG21	1:D:221:ILE:CG1	2.44	0.47
3:I:122:VAL:HG22	3:I:292:HIS:CD2	2.50	0.47
1:G:315:ALA:HB2	4:P:24:PHE:CE1	2.48	0.47
3:F:14:LEU:HD23	3:F:17:ILE:HD12	1.96	0.47
1:K:346:VAL:HG22	5:K:501:HEM:C2D	2.49	0.47
1:K:57:ARG:NH2	5:K:502:HEM:O2D	2.47	0.47
3:M:44:PHE:O	3:M:47:ILE:N	2.47	0.47
1:K:227:PRO:HB3	3:M:47:ILE:HG21	1.95	0.47
1:A:346:VAL:HG22	5:A:501:HEM:C3D	2.49	0.47
1:D:346:VAL:HG22	5:D:501:HEM:C3D	2.49	0.47
1:K:376:HIS:H	1:K:458:THR:HG22	1.80	0.47
2:B:137:MET:HB2	10:B:301:HEC:C1D	2.44	0.47
2:E:62:ARG:HH22	2:E:184:GLU:CD	2.18	0.47
3:I:187:PRO:HG2	3:I:189:TRP:CZ2	2.49	0.47
1:K:359:ILE:HD11	1:K:448:MET:CE	2.44	0.47
1:A:236:SER:HA	3:C:52:ASN:HB2	1.97	0.47
2:H:152:ASP:HA	2:H:155:LYS:HE3	1.95	0.47
2:L:86:TYR:OH	3:M:96:GLU:OE1	2.17	0.47
1:D:228:LYS:HA	3:F:47:ILE:HD11	1.95	0.47
1:G:253:TRP:CH2	3:I:13:THR:HA	2.49	0.47
1:G:94:LEU:O	1:G:98:THR:HG23	2.13	0.47
1:K:226:VAL:HB	1:K:227:PRO:HD3	1.96	0.47
1:K:359:ILE:HD11	1:K:448:MET:HE1	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:446:ALA:O	1:K:450:VAL:HG23	2.15	0.47
3:M:166:ARG:NH2	3:M:250:PRO:HG3	2.30	0.47
1:D:412:ALA:HA	4:O:2:PHE:CD2	2.50	0.47
3:C:270:THR:HG23	3:C:275:ARG:HG2	1.97	0.47
1:D:230:ALA:O	1:D:300:LYS:NZ	2.38	0.47
1:G:250:VAL:HG11	1:G:278:ILE:HG22	1.97	0.47
1:G:310:LEU:O	1:G:313:SER:HB3	2.14	0.47
1:G:359:ILE:HD11	1:G:448:MET:CE	2.43	0.47
1:K:81:VAL:HG23	1:K:161:ASN:ND2	2.29	0.47
2:L:161:ARG:HA	2:L:165:VAL:O	2.15	0.47
1:A:128:TRP:CG	1:A:129:PRO:HD3	2.49	0.47
1:G:233:PRO:CG	3:I:50:TYR:CE2	2.93	0.47
1:K:453:TYR:O	1:K:457:ARG:HG2	2.15	0.47
1:K:82:GLN:CD	1:K:89:LEU:HG	2.35	0.47
2:L:62:ARG:HG3	2:L:63:GLU:N	2.29	0.47
3:F:120:MET:HB3	3:F:120:MET:HE2	1.83	0.47
3:F:68:PHE:O	3:F:68:PHE:HD1	1.98	0.47
2:H:62:ARG:NH1	2:H:63:GLU:OE2	2.48	0.47
3:M:184:ALA:HB1	10:M:402:HEC:HMD1	1.97	0.47
4:P:23:GLY:O	4:P:27:PHE:HB2	2.14	0.47
1:A:376:HIS:CB	1:A:458:THR:HG22	2.44	0.47
1:D:253:TRP:HZ3	3:F:13:THR:HG22	1.79	0.47
3:I:189:TRP:O	3:I:193:ILE:HG22	2.15	0.47
3:I:73:LEU:CD1	3:I:79:LEU:HG	2.45	0.47
1:K:463:LYS:HB2	1:K:464:PRO:CD	2.45	0.47
1:K:252:ILE:HD11	2:L:22:VAL:HG22	1.97	0.47
1:A:76:THR:HG21	1:A:221:ILE:CG1	2.43	0.46
1:K:287:MET:HG3	1:K:288:ILE:N	2.30	0.46
2:L:140:TYR:CE1	10:L:301:HEC:HBB2	2.50	0.46
3:M:157:PHE:HA	3:M:158:PRO:HD3	1.81	0.46
1:D:350:ALA:HB1	5:D:502:HEM:CAC	2.45	0.46
3:F:215:PRO:HB3	11:I:401:FC6:N24	2.30	0.46
3:C:179:LEU:HD22	3:C:283:GLN:HB2	1.97	0.46
1:D:124:ALA:HB2	1:D:205:TYR:CE2	2.51	0.46
2:E:63:GLU:HB3	10:E:301:HEC:HBB1	1.97	0.46
1:G:13:VAL:HA	1:G:16:GLN:HE21	1.79	0.46
3:I:24:ILE:HD13	3:I:24:ILE:C	2.35	0.46
1:K:156:HIS:ND1	2:L:8:GLU:OE2	2.49	0.46
1:A:242:VAL:HG21	3:C:54:LEU:HD21	1.98	0.46
3:F:32:SER:HB3	3:F:36:THR:OG1	2.14	0.46
1:G:350:ALA:HB1	5:G:502:HEM:CAC	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:57:TRP:CG	3:M:58:TRP:N	2.83	0.46
4:Q:20:PHE:C	4:Q:20:PHE:CD2	2.88	0.46
3:F:133:LYS:HD2	3:F:133:LYS:HA	1.76	0.46
2:H:161:ARG:HA	2:H:165:VAL:O	2.15	0.46
11:F:403:FC6:C21	3:I:215:PRO:HG3	2.45	0.46
4:P:13:THR:O	4:P:17:MET:HG2	2.16	0.46
1:A:238:ARG:HH22	3:C:30:GLY:C	2.17	0.46
1:D:57:ARG:NH1	5:D:502:HEM:O2A	2.48	0.46
3:F:86:LEU:HG	3:F:87:PRO:CD	2.39	0.46
3:I:6:SER:HB2	3:I:81:ASN:ND2	2.24	0.46
4:Q:21:LEU:HD13	4:Q:21:LEU:HA	1.60	0.46
3:C:50:TYR:HB3	3:C:52:ASN:ND2	2.31	0.46
1:D:415:ASP:O	3:F:110:TYR:HE2	1.98	0.46
3:I:89:TYR:CZ	3:I:101:ARG:HD2	2.50	0.46
1:K:174:LEU:HD21	1:K:208:ASN:HB3	1.97	0.46
3:M:236:CYS:O	3:M:244:MET:HG3	2.15	0.46
3:F:17:ILE:HA	3:F:20:LEU:HG	1.98	0.46
1:G:227:PRO:HB2	3:I:47:ILE:HG23	1.96	0.46
1:K:228:LYS:CA	3:M:47:ILE:HD11	2.45	0.46
3:M:2:SER:OG	3:M:5:TRP:CD1	2.66	0.46
1:A:66:PHE:O	1:A:70:GLY:HA3	2.16	0.46
2:B:113:GLY:O	2:B:193:GLN:NE2	2.49	0.46
1:K:42:PRO:HG3	2:L:136:LYS:HD2	1.97	0.46
3:M:105:GLN:HB3	3:M:109:LYS:HZ1	1.81	0.46
3:C:85:VAL:HG12	3:C:85:VAL:O	2.15	0.46
1:D:226:VAL:HB	1:D:227:PRO:HD3	1.97	0.46
3:F:57:TRP:HZ3	3:F:61:LEU:HD12	1.80	0.46
2:H:137:MET:HB2	10:H:301:HEC:CHD	2.46	0.46
1:K:196:ALA:HB3	2:L:39:VAL:HB	1.97	0.46
1:K:359:ILE:HD12	1:K:384:HIS:CE1	2.50	0.46
1:K:234:VAL:N	3:M:48:GLU:O	2.49	0.46
1:A:57:ARG:NH1	5:A:502:HEM:HAA1	2.31	0.45
2:B:125:LEU:HD21	10:B:301:HEC:HMB2	1.98	0.45
1:A:250:VAL:CG2	3:C:20:LEU:HD11	2.46	0.45
1:D:455:THR:HG22	1:D:459:VAL:CG2	2.46	0.45
3:F:207:LYS:HA	3:F:212:LEU:O	2.15	0.45
2:E:86:TYR:HE2	3:F:99:TRP:CZ3	2.33	0.45
1:G:321:THR:HG22	5:G:501:HEM:HAB	1.98	0.45
2:L:72:MET:HE3	2:L:100:TRP:CD2	2.50	0.45
1:A:264:LEU:HD12	1:A:265:PRO:HD2	1.97	0.45
1:A:242:VAL:HG22	3:C:27:THR:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:8:TYR:CE2	3:F:12:LEU:HD13	2.52	0.45
3:I:24:ILE:HD12	3:I:59:PHE:CE2	2.48	0.45
3:I:98:GLN:O	3:I:101:ARG:HB2	2.17	0.45
1:A:350:ALA:HB1	5:A:502:HEM:CAC	2.47	0.45
3:F:122:VAL:HG22	3:F:292:HIS:NE2	2.30	0.45
2:H:137:MET:HB2	10:H:301:HEC:C1D	2.47	0.45
3:I:140:ALA:HA	3:I:144:SER:HB3	1.99	0.45
1:A:250:VAL:HG11	1:A:278:ILE:HG22	1.99	0.45
1:D:128:TRP:CG	1:D:129:PRO:HD3	2.51	0.45
2:H:62:ARG:HH22	2:H:184:GLU:CD	2.20	0.45
1:K:12:LYS:HA	1:K:15:ARG:NH1	2.31	0.45
1:K:317:TYR:HB2	1:K:353:TRP:CE3	2.51	0.45
2:B:57:ARG:NH1	2:B:99:LEU:HD12	2.31	0.45
1:D:174:LEU:HD21	1:D:208:ASN:HB3	1.98	0.45
1:D:379:GLY:O	1:D:383:THR:HG23	2.17	0.45
1:D:416:ASP:HA	3:F:110:TYR:HE2	1.81	0.45
1:D:414:ASN:HD21	1:D:420:THR:HG23	1.81	0.45
1:G:156:HIS:HD2	3:I:42:HIS:CD2	2.33	0.45
3:M:167:TRP:CD2	3:M:182:ARG:HG2	2.50	0.45
1:K:224:TYR:HE1	3:M:45:ASP:OD2	2.00	0.45
1:A:152:ARG:NH2	2:B:9:LYS:O	2.50	0.45
1:A:82:GLN:HE21	1:A:88:THR:HA	1.82	0.45
3:C:177:SER:OG	3:C:182:ARG:NH1	2.45	0.45
3:C:4:PHE:CD2	3:C:4:PHE:C	2.89	0.45
1:D:237:TYR:CE2	1:D:241:ILE:HD11	2.51	0.45
1:D:376:HIS:CG	1:D:457:ARG:HB2	2.51	0.45
3:F:236:CYS:O	3:F:244:MET:HG3	2.17	0.45
3:F:28:ARG:HD3	3:F:28:ARG:O	2.16	0.45
3:I:184:ALA:HB1	10:I:402:HEC:HMD1	1.99	0.45
1:K:346:VAL:HG22	5:K:501:HEM:C3D	2.52	0.45
1:A:233:PRO:HG2	3:C:50:TYR:CZ	2.51	0.45
1:D:287:MET:HG3	1:D:288:ILE:N	2.31	0.45
1:K:115:LEU:HB3	1:K:117:PHE:CE2	2.51	0.45
1:K:308:ARG:NH1	1:K:382:ASN:HD21	2.14	0.45
3:M:73:LEU:CD2	3:M:79:LEU:HD11	2.46	0.45
1:A:336:SER:O	1:A:339:THR:OG1	2.17	0.45
2:B:109:LEU:O	2:B:112:VAL:HG22	2.17	0.45
2:B:140:TYR:CE1	10:B:301:HEC:HBB2	2.51	0.45
3:F:135:GLY:HA3	3:F:297:TYR:HB2	1.99	0.45
1:D:158:TYR:HB2	3:F:44:PHE:CD2	2.51	0.45
3:F:67:VAL:O	3:F:71:LEU:HD13	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:301:LEU:HD21	1:K:311:VAL:HG21	1.98	0.45
1:K:233:PRO:HG2	3:M:50:TYR:CE2	2.51	0.45
1:A:253:TRP:CH2	3:C:13:THR:HA	2.52	0.45
3:C:31:GLU:HG3	3:C:53:PRO:HB3	1.99	0.45
1:D:82:GLN:HE21	1:D:89:LEU:H	1.65	0.45
1:G:309:PHE:CE2	1:G:359:ILE:HG21	2.52	0.45
1:A:159:VAL:HA	1:A:162:TRP:CD2	2.52	0.45
1:A:73:LEU:HD12	1:A:73:LEU:HA	1.81	0.45
1:D:81:VAL:HG23	1:D:161:ASN:ND2	2.32	0.45
2:E:137:MET:HB2	10:E:301:HEC:C1D	2.47	0.45
1:G:212:PHE:HA	1:G:216:ALA:HB3	1.99	0.45
3:I:186:MET:HG2	10:I:402:HEC:C1D	2.44	0.45
3:M:270:THR:HG23	3:M:275:ARG:HG2	1.98	0.45
1:G:128:TRP:CG	1:G:129:PRO:HD3	2.52	0.44
1:G:82:GLN:HE21	1:G:89:LEU:H	1.65	0.44
3:I:255:ALA:HA	3:I:258:TRP:CD2	2.51	0.44
1:K:235:TYR:CE2	1:K:292:MET:HB2	2.51	0.44
1:K:355:ALA:O	1:K:359:ILE:HG12	2.16	0.44
3:M:43:ALA:CB	3:M:48:GLU:HB3	2.46	0.44
3:M:40:MET:HG2	3:M:51:ASP:HB2	1.98	0.44
1:A:238:ARG:O	1:A:242:VAL:HG23	2.18	0.44
1:A:291:MET:SD	4:N:24:PHE:HZ	2.40	0.44
2:B:88:VAL:HG12	2:B:90:GLY:H	1.82	0.44
1:D:115:LEU:HB3	1:D:117:PHE:CE2	2.51	0.44
1:D:267:TRP:HB2	3:F:78:GLY:O	2.17	0.44
1:D:443:ILE:O	1:D:446:ALA:HB3	2.17	0.44
5:D:501:HEM:HBB2	5:D:501:HEM:HMB1	1.98	0.44
3:F:4:PHE:C	3:F:4:PHE:CD1	2.90	0.44
3:M:205:VAL:HG21	10:M:402:HEC:HMB3	1.99	0.44
1:K:411:ARG:NH1	4:Q:4:ASP:OD2	2.51	0.44
3:C:36:THR:HG22	3:C:38:GLN:HG2	1.99	0.44
2:E:109:LEU:O	2:E:112:VAL:HG22	2.18	0.44
10:F:401:HEC:HMC1	10:F:401:HEC:HBC3	1.99	0.44
3:F:68:PHE:HA	3:F:71:LEU:HD22	1.99	0.44
3:I:121:SER:O	3:I:125:VAL:HG23	2.16	0.44
9:K:506:PO4:P	3:M:72:TYR:OH	2.75	0.44
10:C:402:HEC:HMC1	10:C:402:HEC:HBC3	1.98	0.44
1:D:11:TYR:CD1	1:D:369:VAL:HA	2.53	0.44
1:D:64:VAL:HG11	5:D:502:HEM:C4C	2.53	0.44
3:F:73:LEU:HB3	3:F:79:LEU:CD1	2.43	0.44
1:G:82:GLN:HE21	1:G:88:THR:HA	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:90:PHE:CD1	1:K:147:GLY:CA	3.01	0.44
3:M:56:ARG:O	3:M:59:PHE:HB3	2.17	0.44
1:A:207:HIS:CD2	1:A:251:TYR:HD1	2.33	0.44
1:A:226:VAL:HB	1:A:227:PRO:HD3	1.99	0.44
2:B:62:ARG:HH22	2:B:184:GLU:CD	2.20	0.44
1:D:174:LEU:HD12	1:D:204:TRP:CZ2	2.52	0.44
3:F:121:SER:C	3:F:125:VAL:HG23	2.37	0.44
3:F:38:GLN:CA	3:F:38:GLN:HE21	2.29	0.44
3:F:89:TYR:CD1	3:F:93:TRP:HD1	2.36	0.44
1:G:367:PRO:HD3	1:G:375:MET:HE3	1.99	0.44
1:K:384:HIS:CE1	1:K:451:MET:HB2	2.52	0.44
2:L:152:ASP:HA	2:L:155:LYS:HE3	1.98	0.44
3:M:38:GLN:O	3:M:50:TYR:CE2	2.71	0.44
1:A:305:PRO:HB2	1:A:381:ILE:HG22	1.98	0.44
1:G:264:LEU:HD12	1:G:265:PRO:HD2	1.99	0.44
1:G:377:SER:H	1:G:454:ASN:HD21	1.66	0.44
1:G:76:THR:HG21	1:G:221:ILE:CG1	2.45	0.44
1:G:261:TYR:HA	3:I:95:GLN:OE1	2.18	0.44
2:L:148:LEU:HD11	2:L:187:ALA:HB2	2.00	0.44
1:G:340:ASP:H	1:G:406:GLN:HE22	1.65	0.44
2:L:129:ARG:HD3	2:L:135:SER:O	2.18	0.44
1:D:331:THR:O	4:O:6:VAL:HG13	2.18	0.44
4:Q:4:ASP:H	4:Q:7:VAL:HB	1.82	0.44
1:A:39:LEU:HA	1:A:39:LEU:HD23	1.88	0.44
3:C:121:SER:O	3:C:125:VAL:HG23	2.18	0.44
3:C:242:GLU:CD	3:C:242:GLU:H	2.20	0.44
5:G:501:HEM:HBB2	5:G:501:HEM:HMB1	1.99	0.44
1:A:81:VAL:HG23	1:A:161:ASN:ND2	2.33	0.44
3:C:157:PHE:HA	3:C:158:PRO:HD3	1.83	0.44
2:E:80:THR:HA	2:E:84:GLY:O	2.18	0.44
3:F:88:GLY:O	3:F:89:TYR:HD2	2.01	0.44
1:G:108:LEU:HA	1:G:108:LEU:HD12	1.80	0.44
1:G:305:PRO:HB2	1:G:381:ILE:HG22	2.00	0.44
1:K:76:THR:HG21	1:K:221:ILE:CG1	2.46	0.44
3:M:189:TRP:O	3:M:193:ILE:HG22	2.16	0.44
3:F:82:TRP:HD1	3:F:82:TRP:C	2.19	0.43
1:K:11:TYR:CD1	1:K:369:VAL:HA	2.53	0.43
3:M:140:ALA:HA	3:M:144:SER:HB3	2.00	0.43
3:C:140:ALA:O	3:C:144:SER:OG	2.21	0.43
1:D:170:THR:HB	2:E:22:VAL:HG21	1.99	0.43
1:D:182:ILE:HD12	2:E:163:LEU:HG	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:111:ARG:HH22	2:E:199:LEU:HD13	1.83	0.43
2:E:161:ARG:HA	2:E:165:VAL:O	2.19	0.43
1:K:379:GLY:O	1:K:383:THR:HG23	2.17	0.43
2:L:51:ALA:HB1	2:L:153:THR:HG21	1.99	0.43
4:P:4:ASP:H	4:P:7:VAL:HB	1.83	0.43
1:A:235:TYR:CD1	1:A:236:SER:HB2	2.54	0.43
1:A:350:ALA:HB1	5:A:502:HEM:C3C	2.54	0.43
1:D:321:THR:HG22	5:D:501:HEM:HAB	2.00	0.43
1:K:235:TYR:CD2	1:K:292:MET:CB	3.01	0.43
1:K:377:SER:H	1:K:454:ASN:HD21	1.67	0.43
1:K:376:HIS:HB3	1:K:454:ASN:ND2	2.32	0.43
2:B:6:LYS:HD2	2:B:6:LYS:HA	1.61	0.43
3:C:74:VAL:O	3:C:82:TRP:HH2	2.02	0.43
1:D:264:LEU:HD12	1:D:265:PRO:HD2	1.99	0.43
1:D:384:HIS:HE1	1:D:451:MET:HE3	1.83	0.43
3:F:114:PHE:CD1	3:F:289:ASP:HB3	2.53	0.43
3:F:83:LYS:HD2	3:F:91:GLY:O	2.17	0.43
1:G:35:ILE:HB	1:G:53:PHE:CE1	2.54	0.43
3:I:121:SER:OG	3:I:123:GLU:HG2	2.19	0.43
3:M:38:GLN:HB2	3:M:39:THR:H	1.64	0.43
4:O:20:PHE:CD2	4:O:20:PHE:C	2.92	0.43
4:O:26:TYR:N	4:O:26:TYR:CD2	2.86	0.43
1:D:207:HIS:CD2	1:D:251:TYR:HD1	2.36	0.43
1:D:463:LYS:H	1:D:463:LYS:HG2	1.59	0.43
1:G:354:VAL:O	1:G:358:SER:OG	2.30	0.43
1:K:124:ALA:HB2	1:K:205:TYR:CE2	2.52	0.43
1:K:305:PRO:O	1:K:308:ARG:HB2	2.18	0.43
2:L:42:PRO:HG3	2:L:93:VAL:HG11	2.00	0.43
3:M:89:TYR:HA	3:M:101:ARG:NH2	2.33	0.43
4:P:4:ASP:OD1	4:P:5:ASN:N	2.48	0.43
1:D:92:PRO:O	1:D:95:ALA:HB3	2.18	0.43
1:D:238:ARG:NH1	3:F:30:GLY:O	2.52	0.43
3:I:205:VAL:HG21	10:I:402:HEC:HMB3	2.01	0.43
1:K:233:PRO:CG	3:M:50:TYR:CE2	3.02	0.43
1:K:309:PHE:CE2	1:K:359:ILE:HG21	2.54	0.43
1:K:446:ALA:HA	1:K:449:LEU:HD12	2.00	0.43
3:M:60:LEU:HD13	3:M:61:LEU:N	2.34	0.43
1:A:410:TRP:O	2:B:82:ARG:NH1	2.52	0.43
1:A:457:ARG:HH11	1:A:457:ARG:HD2	1.67	0.43
3:C:206:ARG:HG2	3:C:212:LEU:HB2	2.01	0.43
3:F:120:MET:HE1	3:F:124:GLU:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:258:TRP:CZ3	3:F:267:LEU:HD21	2.54	0.43
1:G:346:VAL:HG22	5:G:501:HEM:C3D	2.53	0.43
1:G:371:GLY:HA3	1:G:465:ALA:HB1	1.99	0.43
3:I:57:TRP:CG	3:I:58:TRP:N	2.86	0.43
3:M:77:PRO:HG3	3:M:93:TRP:O	2.19	0.43
3:C:20:LEU:HD23	3:C:20:LEU:HA	1.78	0.43
3:C:45:ASP:CG	3:C:46:GLY:H	2.22	0.43
3:C:50:TYR:HB2	3:C:52:ASN:HD22	1.84	0.43
1:D:108:LEU:HA	1:D:108:LEU:HD12	1.81	0.43
1:D:376:HIS:CE1	1:D:457:ARG:HG3	2.54	0.43
1:D:350:ALA:HB1	5:D:502:HEM:C3C	2.54	0.43
3:F:58:TRP:CH2	3:F:62:PHE:HD2	2.37	0.43
1:G:207:HIS:CD2	1:G:251:TYR:HD1	2.36	0.43
3:I:85:VAL:O	3:I:85:VAL:HG12	2.19	0.43
1:K:128:TRP:CG	1:K:129:PRO:HD3	2.54	0.43
1:K:159:VAL:HA	1:K:162:TRP:CD2	2.54	0.43
1:A:343:ILE:HG12	5:A:502:HEM:HBA2	2.01	0.43
1:A:55:ARG:HH21	2:B:63:GLU:CD	2.22	0.43
2:E:51:ALA:HB1	2:E:153:THR:HG21	2.01	0.43
3:F:206:ARG:HG2	3:F:212:LEU:HB2	2.00	0.43
3:F:37:ASP:HB2	3:F:38:GLN:NE2	2.34	0.43
3:I:229:TYR:HE1	3:I:239:GLN:HA	1.83	0.43
3:I:279:MET:HB2	10:I:403:HEC:C4D	2.48	0.43
1:G:228:LYS:NZ	3:I:45:ASP:OD1	2.46	0.43
3:I:24:ILE:CD1	3:I:59:PHE:HE2	2.31	0.43
1:K:463:LYS:CB	1:K:464:PRO:CD	2.95	0.43
3:M:279:MET:HB2	10:M:403:HEC:C4D	2.48	0.43
1:A:266:ASP:OD2	3:C:95:GLN:HG2	2.19	0.43
1:A:319:MET:HG3	1:A:320:SER:N	2.34	0.43
1:A:327:MET:HE2	1:A:327:MET:HB2	1.86	0.43
3:C:264:LEU:O	3:C:268:GLN:HG3	2.19	0.43
1:D:260:HIS:HB2	1:D:333:ASN:OD1	2.19	0.43
1:D:335:LEU:HD13	4:O:7:VAL:HA	2.00	0.43
1:D:158:TYR:HE2	3:F:49:GLU:OE2	2.02	0.43
1:G:446:ALA:O	1:G:450:VAL:HG23	2.19	0.43
3:I:24:ILE:CD1	3:I:59:PHE:CE2	3.02	0.43
1:K:125:GLU:HG2	1:K:125:GLU:H	1.42	0.43
2:L:140:TYR:OH	10:L:301:HEC:HMC2	2.19	0.43
1:A:195:GLY:HA2	2:B:92:SER:HB2	2.00	0.42
1:D:308:ARG:NH1	1:D:382:ASN:HD21	2.17	0.42
2:E:116:TYR:HE2	3:F:145:ILE:HG21	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:279:MET:HB2	10:F:402:HEC:C4D	2.49	0.42
3:F:60:LEU:HA	3:F:60:LEU:HD23	1.74	0.42
3:I:206:ARG:HG2	3:I:212:LEU:HB2	2.01	0.42
3:I:50:TYR:CB	3:I:52:ASN:OD1	2.64	0.42
3:I:63:ILE:N	3:I:63:ILE:HD13	2.34	0.42
1:A:196:ALA:HB3	2:B:39:VAL:HB	2.02	0.42
2:E:62:ARG:HG3	2:E:63:GLU:N	2.34	0.42
3:F:103:VAL:HG12	3:F:107:ASP:OD2	2.19	0.42
1:G:235:TYR:CD1	1:G:236:SER:HB2	2.53	0.42
3:C:177:SER:HA	3:C:182:ARG:HD2	2.02	0.42
3:C:59:PHE:CD1	3:C:63:ILE:HD11	2.53	0.42
1:D:13:VAL:HA	1:D:16:GLN:NE2	2.35	0.42
1:D:349:GLY:O	1:D:353:TRP:HB3	2.20	0.42
3:F:179:LEU:HD22	3:F:283:GLN:HB2	2.00	0.42
2:H:7:LEU:HA	2:H:10:ASN:ND2	2.30	0.42
2:H:80:THR:HA	2:H:84:GLY:O	2.19	0.42
3:I:179:LEU:HD22	3:I:283:GLN:HB2	2.01	0.42
3:I:24:ILE:HD11	3:I:59:PHE:CD2	2.54	0.42
3:I:94:THR:OG1	3:I:97:LYS:HG3	2.19	0.42
1:K:305:PRO:HA	1:K:308:ARG:HB2	2.01	0.42
1:A:125:GLU:HG2	1:A:125:GLU:H	1.30	0.42
1:A:235:TYR:CE1	1:A:236:SER:HB2	2.53	0.42
1:A:301:LEU:HD21	1:A:311:VAL:HG21	2.01	0.42
1:A:218:PHE:CZ	1:A:354:VAL:HG13	2.54	0.42
1:A:454:ASN:O	1:A:458:THR:HG23	2.19	0.42
1:D:317:TYR:HB2	1:D:353:TRP:CE3	2.55	0.42
1:G:226:VAL:HB	1:G:227:PRO:HD3	2.01	0.42
3:I:157:PHE:HA	3:I:158:PRO:HD3	1.81	0.42
3:I:75:LEU:HD22	3:I:86:LEU:HB2	2.01	0.42
1:A:317:TYR:HB2	1:A:353:TRP:CE3	2.54	0.42
1:A:395:TYR:CZ	1:A:437:ARG:HD2	2.55	0.42
3:F:144:SER:O	3:F:148:GLY:N	2.52	0.42
2:H:116:TYR:HE2	3:I:145:ILE:HG21	1.83	0.42
1:K:227:PRO:HB2	3:M:47:ILE:HG12	2.02	0.42
10:F:402:HEC:HBC3	10:F:402:HEC:HMC1	2.00	0.42
1:G:208:ASN:OD1	1:G:252:ILE:HA	2.20	0.42
3:I:297:TYR:CZ	3:I:301:LEU:HD11	2.55	0.42
1:K:279:LEU:O	1:K:282:PRO:HD2	2.19	0.42
1:K:228:LYS:NZ	3:M:46:GLY:HA3	2.33	0.42
3:M:68:PHE:CA	3:M:71:LEU:HD12	2.36	0.42
3:M:90:GLU:O	3:M:97:LYS:NZ	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:232:THR:HB	10:C:401:HEC:HBB1	2.02	0.42
1:D:279:LEU:O	1:D:282:PRO:HD2	2.19	0.42
1:D:457:ARG:HA	1:D:457:ARG:HD2	1.84	0.42
1:G:375:MET:HG3	1:G:381:ILE:HD11	2.01	0.42
1:G:58:PRO:HA	1:G:61:THR:HB	2.01	0.42
2:H:24:ILE:HG21	3:I:16:THR:HG23	2.01	0.42
1:K:349:GLY:O	1:K:353:TRP:HB3	2.19	0.42
4:N:4:ASP:OD1	4:N:5:ASN:N	2.48	0.42
3:C:89:TYR:CD1	3:C:93:TRP:CD1	3.07	0.42
1:D:309:PHE:CE2	1:D:359:ILE:HG21	2.55	0.42
1:K:254:ALA:O	1:K:257:HIS:ND1	2.52	0.42
4:Q:4:ASP:OD1	4:Q:5:ASN:N	2.50	0.42
1:A:308:ARG:NH1	1:A:382:ASN:HD21	2.18	0.42
1:D:62:ASN:ND2	1:D:125:GLU:HG3	2.35	0.42
1:D:305:PRO:HB2	1:D:381:ILE:HG22	2.02	0.42
1:D:253:TRP:CH2	3:F:13:THR:HA	2.54	0.42
3:M:271:ILE:HG12	10:M:402:HEC:HMB2	2.02	0.42
1:A:375:MET:HA	1:A:375:MET:HE2	2.02	0.42
2:B:80:THR:HA	2:B:84:GLY:O	2.20	0.42
3:C:177:SER:HB2	10:C:402:HEC:HMA2	2.02	0.42
3:C:50:TYR:HB2	3:C:52:ASN:ND2	2.35	0.42
1:D:307:LEU:HA	1:D:307:LEU:HD12	1.94	0.42
2:E:56:GLY:HA2	2:E:59:LEU:HD12	2.01	0.42
3:F:270:THR:HG23	3:F:275:ARG:HG2	2.01	0.42
1:G:340:ASP:H	1:G:406:GLN:NE2	2.18	0.42
1:G:57:ARG:NH2	5:G:502:HEM:O2D	2.52	0.42
1:G:81:VAL:HA	1:G:84:THR:HG22	2.02	0.42
1:A:466:GLU:OE1	1:A:466:GLU:HA	2.20	0.41
2:B:193:GLN:HA	2:B:193:GLN:NE2	2.34	0.41
3:F:189:TRP:O	3:F:193:ILE:HG22	2.19	0.41
1:K:208:ASN:OD1	1:K:252:ILE:HA	2.20	0.41
1:A:57:ARG:NH2	5:A:502:HEM:O2D	2.53	0.41
2:B:42:PRO:HG3	2:B:93:VAL:HG11	2.02	0.41
3:C:22:TRP:CE3	3:C:23:LEU:HA	2.54	0.41
3:C:35:THR:O	3:C:52:ASN:OD1	2.37	0.41
1:D:82:GLN:HE21	1:D:88:THR:HA	1.85	0.41
3:F:240:GLY:O	3:F:253:ASN:HB3	2.20	0.41
1:K:263:ALA:HB3	2:L:100:TRP:CH2	2.54	0.41
2:B:137:MET:HA	2:B:138:PRO:HD3	1.95	0.41
3:C:212:LEU:HA	3:C:212:LEU:HD23	1.85	0.41
1:G:182:ILE:HD12	2:H:163:LEU:HG	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:13:VAL:HA	1:K:16:GLN:NE2	2.34	0.41
3:M:136:ALA:HB2	3:M:297:TYR:CE1	2.54	0.41
1:G:411:ARG:NH1	4:P:4:ASP:OD2	2.51	0.41
1:A:108:LEU:HA	1:A:108:LEU:HD12	1.78	0.41
1:G:10:SER:HB2	1:G:88:THR:HG23	2.02	0.41
1:G:218:PHE:CD2	1:G:221:ILE:HD12	2.56	0.41
1:G:319:MET:HG3	1:G:320:SER:N	2.35	0.41
3:I:24:ILE:HD13	3:I:24:ILE:O	2.20	0.41
3:M:9:ILE:HD12	3:M:80:GLY:HA2	2.02	0.41
1:A:12:LYS:HA	1:A:15:ARG:NH1	2.34	0.41
1:D:94:LEU:O	1:D:98:THR:HG23	2.19	0.41
2:E:137:MET:HB2	10:E:301:HEC:CHD	2.50	0.41
3:F:17:ILE:HA	3:F:20:LEU:CG	2.50	0.41
3:F:89:TYR:HB3	3:F:97:LYS:NZ	2.35	0.41
1:G:159:VAL:HA	1:G:162:TRP:CG	2.55	0.41
1:K:115:LEU:HD23	1:K:117:PHE:HE2	1.86	0.41
1:K:17:PHE:O	1:K:21:THR:OG1	2.33	0.41
3:M:24:ILE:CD1	3:M:59:PHE:HE2	2.33	0.41
1:D:305:PRO:HA	1:D:308:ARG:HB2	2.03	0.41
3:F:111:GLY:N	3:F:112:PRO:CD	2.83	0.41
3:F:37:ASP:HB3	3:F:38:GLN:CA	2.32	0.41
1:G:218:PHE:CZ	1:G:354:VAL:HG13	2.56	0.41
2:H:125:LEU:HD21	10:H:301:HEC:HMB2	2.02	0.41
2:H:7:LEU:HG	2:H:7:LEU:O	2.20	0.41
1:K:193:TYR:CE1	1:K:201:VAL:HG11	2.55	0.41
1:K:218:PHE:CD2	1:K:221:ILE:HD12	2.55	0.41
1:K:66:PHE:O	1:K:70:GLY:HA3	2.20	0.41
1:K:84:THR:O	3:M:44:PHE:CE2	2.74	0.41
3:C:40:MET:HB2	3:C:40:MET:HE3	1.99	0.41
1:D:235:TYR:CD1	1:D:236:SER:HB2	2.56	0.41
2:E:148:LEU:HD11	2:E:187:ALA:HB2	2.02	0.41
3:F:122:VAL:HA	3:F:125:VAL:HG23	2.03	0.41
3:F:139:PHE:CD1	3:F:143:CYS:HB2	2.56	0.41
3:F:40:MET:CB	3:F:49:GLU:HB2	2.50	0.41
1:G:174:LEU:HD21	1:G:208:ASN:HB3	2.02	0.41
1:G:294:LEU:HD11	1:G:307:LEU:HD11	2.03	0.41
1:G:64:VAL:HG21	5:G:502:HEM:C2C	2.55	0.41
1:G:66:PHE:O	1:G:70:GLY:HA3	2.21	0.41
3:M:215:PRO:CD	3:M:264:LEU:HD12	2.51	0.41
2:B:128:PRO:HD3	2:B:139:SER:HA	2.03	0.41
1:D:237:TYR:O	1:D:241:ILE:HD12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:85:VAL:O	3:F:85:VAL:HG12	2.21	0.41
3:M:24:ILE:CD1	3:M:59:PHE:CE2	3.01	0.41
1:A:58:PRO:HA	1:A:61:THR:HB	2.03	0.41
3:F:157:PHE:HA	3:F:158:PRO:HD3	1.80	0.41
3:F:271:ILE:CD1	10:F:401:HEC:HMB2	2.51	0.41
2:H:96:HIS:HA	2:H:97:PRO:HA	1.87	0.41
2:L:96:HIS:HA	2:L:97:PRO:HA	1.88	0.41
3:M:207:LYS:HA	3:M:212:LEU:O	2.21	0.41
3:M:61:LEU:HD12	3:M:61:LEU:HA	1.91	0.41
4:N:20:PHE:C	4:N:20:PHE:CD2	2.95	0.41
1:A:431:HIS:HD2	2:B:136:LYS:NZ	2.18	0.41
1:D:195:GLY:HA2	2:E:92:SER:HB2	2.02	0.41
3:F:134:MET:HG2	3:F:293:LEU:HD13	2.03	0.41
3:F:89:TYR:HB3	3:F:97:LYS:HZ3	1.86	0.41
1:G:290:GLY:O	1:G:293:THR:HB	2.21	0.41
1:G:418:THR:OG1	3:I:137:ARG:NH1	2.54	0.41
10:I:403:HEC:HBC3	10:I:403:HEC:HMC1	2.03	0.41
1:G:233:PRO:HB3	3:I:48:GLU:HG3	2.03	0.41
3:I:6:SER:CB	3:I:81:ASN:HD22	2.25	0.41
3:M:166:ARG:HH21	10:M:402:HEC:HAD2	1.85	0.41
1:A:218:PHE:CD2	1:A:221:ILE:HD12	2.56	0.41
1:A:82:GLN:HE21	1:A:89:LEU:H	1.67	0.41
3:C:21:PHE:O	3:C:24:ILE:HG22	2.21	0.41
3:C:255:ALA:HA	3:C:258:TRP:CD2	2.56	0.41
3:F:128:ASP:C	3:F:128:ASP:OD2	2.58	0.41
1:G:317:TYR:HB2	1:G:353:TRP:CE3	2.56	0.41
2:H:137:MET:HA	2:H:138:PRO:HD3	1.98	0.41
2:H:74:ARG:HA	2:H:75:PRO:HD3	1.88	0.41
1:K:457:ARG:HA	1:K:457:ARG:HD2	1.76	0.41
3:M:212:LEU:HD23	3:M:212:LEU:HA	1.86	0.41
1:A:81:VAL:HA	1:A:84:THR:HG22	2.03	0.40
3:C:166:ARG:NH2	3:C:250:PRO:HG3	2.37	0.40
11:C:403:FC6:N25	3:M:215:PRO:HG3	2.36	0.40
3:F:14:LEU:O	3:F:17:ILE:HB	2.21	0.40
3:F:255:ALA:HA	3:F:258:TRP:CD2	2.56	0.40
3:F:282:GLN:HB3	3:F:286:LEU:HD12	2.03	0.40
1:K:350:ALA:HB1	5:K:502:HEM:C3C	2.57	0.40
3:M:8:TYR:HA	3:M:11:LEU:HD22	2.02	0.40
1:K:267:TRP:CA	3:M:78:GLY:HA2	2.48	0.40
1:A:174:LEU:HD21	1:A:208:ASN:HB3	2.03	0.40
1:A:291:MET:HE2	1:A:291:MET:HB2	1.76	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:TRP:O	1:A:390:ILE:HG12	2.21	0.40
1:A:77:SER:O	1:A:81:VAL:HG12	2.21	0.40
1:D:237:TYR:O	1:D:240:SER:HB2	2.21	0.40
2:E:96:HIS:HA	2:E:97:PRO:HA	1.90	0.40
3:F:239:GLN:HG3	3:F:239:GLN:O	2.20	0.40
3:I:69:GLY:O	3:I:73:LEU:HD23	2.21	0.40
1:K:57:ARG:NH1	5:K:502:HEM:O2A	2.54	0.40
4:Q:27:PHE:O	4:Q:27:PHE:CD2	2.73	0.40
1:A:13:VAL:HA	1:A:16:GLN:NE2	2.33	0.40
1:A:331:THR:O	4:N:6:VAL:HG13	2.21	0.40
1:A:351:LEU:O	1:A:355:ALA:HB3	2.21	0.40
2:B:48:PRO:HG3	2:B:166:PRO:HD2	2.03	0.40
1:A:288:ILE:HD12	3:C:58:TRP:CD1	2.56	0.40
3:C:57:TRP:CG	3:C:58:TRP:N	2.89	0.40
2:E:125:LEU:HD21	10:E:301:HEC:HMB2	2.02	0.40
1:G:235:TYR:O	1:G:289:ASN:ND2	2.54	0.40
1:G:349:GLY:O	1:G:353:TRP:HB3	2.22	0.40
1:G:11:TYR:CD1	1:G:369:VAL:HA	2.56	0.40
1:G:453:TYR:O	1:G:457:ARG:HG2	2.20	0.40
1:K:90:PHE:C	1:K:90:PHE:CD2	2.95	0.40
3:M:60:LEU:HD22	3:M:60:LEU:O	2.21	0.40
1:A:279:LEU:O	1:A:282:PRO:HD2	2.22	0.40
3:C:47:ILE:H	3:C:47:ILE:HG12	1.69	0.40
1:D:236:SER:OG	1:D:239:LEU:HB2	2.21	0.40
1:D:254:ALA:O	1:D:257:HIS:ND1	2.55	0.40
1:D:395:TYR:CZ	1:D:437:ARG:HD2	2.57	0.40
3:F:61:LEU:O	3:F:65:THR:HG23	2.20	0.40
1:G:256:PRO:HB2	1:G:272:GLY:HA3	2.03	0.40
1:G:379:GLY:O	1:G:383:THR:HG23	2.22	0.40
3:M:76:TYR:CE1	3:M:86:LEU:HD22	2.57	0.40
1:A:294:LEU:HD11	1:A:307:LEU:HD11	2.04	0.40
2:B:132:VAL:HA	2:B:133:PRO:HD2	1.89	0.40
1:D:253:TRP:CH2	3:F:13:THR:HG22	2.55	0.40
3:F:140:ALA:HA	3:F:144:SER:HB3	2.04	0.40
1:G:386:TRP:O	1:G:390:ILE:HG12	2.21	0.40
1:K:15:ARG:HG3	1:K:369:VAL:HG12	2.03	0.40
2:L:109:LEU:O	2:L:112:VAL:HG22	2.22	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	464/474 (98%)	442 (95%)	20 (4%)	2 (0%)	39	80
1	D	461/474 (97%)	443 (96%)	17 (4%)	1 (0%)	52	88
1	G	463/474 (98%)	443 (96%)	19 (4%)	1 (0%)	52	88
1	K	463/474 (98%)	442 (96%)	19 (4%)	2 (0%)	39	80
2	B	195/203 (96%)	187 (96%)	8 (4%)	0	100	100
2	E	195/203 (96%)	187 (96%)	8 (4%)	0	100	100
2	H	195/203 (96%)	187 (96%)	8 (4%)	0	100	100
2	L	195/203 (96%)	187 (96%)	8 (4%)	0	100	100
3	C	301/311 (97%)	286 (95%)	15 (5%)	0	100	100
3	F	301/311 (97%)	286 (95%)	15 (5%)	0	100	100
3	I	301/311 (97%)	287 (95%)	14 (5%)	0	100	100
3	M	301/311 (97%)	284 (94%)	14 (5%)	3 (1%)	19	65
4	N	27/36 (75%)	27 (100%)	0	0	100	100
4	O	27/36 (75%)	27 (100%)	0	0	100	100
4	P	27/36 (75%)	27 (100%)	0	0	100	100
4	Q	27/36 (75%)	27 (100%)	0	0	100	100
All	All	3943/4096 (96%)	3769 (96%)	165 (4%)	9 (0%)	52	88

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	466	GLU
1	A	468	ASP
1	G	465	ALA
1	K	466	GLU
1	K	468	ASP
3	M	38	GLN

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Mol	Chain	Res	Type
3	M	42	HIS
3	M	37	ASP
1	D	463	LYS

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	374/379 (99%)	343 (92%)	31 (8%)	14 49
1	D	371/379 (98%)	339 (91%)	32 (9%)	13 46
1	G	373/379 (98%)	340 (91%)	33 (9%)	12 45
1	K	373/379 (98%)	339 (91%)	34 (9%)	12 42
2	B	166/172 (96%)	154 (93%)	12 (7%)	18 57
2	E	166/172 (96%)	155 (93%)	11 (7%)	21 61
2	H	166/172 (96%)	152 (92%)	14 (8%)	14 48
2	L	166/172 (96%)	155 (93%)	11 (7%)	21 61
3	C	227/234 (97%)	212 (93%)	15 (7%)	21 61
3	F	227/234 (97%)	197 (87%)	30 (13%)	5 23
3	I	227/234 (97%)	200 (88%)	27 (12%)	6 28
3	M	227/234 (97%)	203 (89%)	24 (11%)	8 34
4	N	22/28 (79%)	22 (100%)	0	100 100
4	O	22/28 (79%)	22 (100%)	0	100 100
4	P	22/28 (79%)	21 (96%)	1 (4%)	34 74
4	Q	22/28 (79%)	19 (86%)	3 (14%)	5 22
All	All	3151/3252 (97%)	2873 (91%)	278 (9%)	12 45

All (278) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	TRP

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Mol	Chain	Res	Type
1	A	57	ARG
1	A	59	LEU
1	A	64	VAL
1	A	73	LEU
1	A	87	THR
1	A	104	LEU
1	A	107	LEU
1	A	108	LEU
1	A	119	SER
1	A	125	GLU
1	A	154	VAL
1	A	159	VAL
1	A	167	PHE
1	A	174	LEU
1	A	192	LEU
1	A	200	MET
1	A	243	HIS
1	A	251	TYR
1	A	271	LEU
1	A	275	MET
1	A	278	ILE
1	A	289	ASN
1	A	294	LEU
1	A	313	SER
1	A	319	MET
1	A	372	ARG
1	A	373	GLU
1	A	427	LEU
1	A	454	ASN
1	A	458	THR
2	B	6	LYS
2	B	13	LEU
2	B	16	LEU
2	B	17	PHE
2	B	22	VAL
2	B	27	LEU
2	B	62	ARG
2	B	92	SER
2	B	112	VAL
2	B	127	ASN
2	B	129	ARG
2	B	177	ASP

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Mol	Chain	Res	Type
3	C	8	TYR
3	C	16	THR
3	C	27	THR
3	C	40	MET
3	C	47	ILE
3	C	48	GLU
3	C	62	PHE
3	C	130	GLN
3	C	163	GLN
3	C	175	LYS
3	C	179	LEU
3	C	182	ARG
3	C	201	VAL
3	C	239	GLN
3	C	264	LEU
1	D	50	TRP
1	D	57	ARG
1	D	59	LEU
1	D	64	VAL
1	D	73	LEU
1	D	87	THR
1	D	93	LYS
1	D	104	LEU
1	D	107	LEU
1	D	108	LEU
1	D	119	SER
1	D	125	GLU
1	D	154	VAL
1	D	159	VAL
1	D	167	PHE
1	D	174	LEU
1	D	192	LEU
1	D	200	MET
1	D	243	HIS
1	D	248	ILE
1	D	251	TYR
1	D	271	LEU
1	D	275	MET
1	D	278	ILE
1	D	289	ASN
1	D	294	LEU
1	D	319	MET

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Mol	Chain	Res	Type
1	D	372	ARG
1	D	373	GLU
1	D	427	LEU
1	D	456	TRP
1	D	467	TYR
2	E	13	LEU
2	E	16	LEU
2	E	17	PHE
2	E	22	VAL
2	E	27	LEU
2	E	62	ARG
2	E	92	SER
2	E	112	VAL
2	E	127	ASN
2	E	129	ARG
2	E	177	ASP
3	F	4	PHE
3	F	8	TYR
3	F	12	LEU
3	F	16	THR
3	F	20	LEU
3	F	21	PHE
3	F	24	ILE
3	F	27	THR
3	F	28	ARG
3	F	29	LYS
3	F	35	THR
3	F	36	THR
3	F	38	GLN
3	F	40	MET
3	F	54	LEU
3	F	62	PHE
3	F	63	ILE
3	F	68	PHE
3	F	71	LEU
3	F	82	TRP
3	F	121	SER
3	F	134	MET
3	F	137	ARG
3	F	145	ILE
3	F	163	GLN
3	F	175	LYS

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Mol	Chain	Res	Type
3	F	179	LEU
3	F	182	ARG
3	F	201	VAL
3	F	264	LEU
1	G	6	SER
1	G	50	TRP
1	G	57	ARG
1	G	59	LEU
1	G	64	VAL
1	G	73	LEU
1	G	87	THR
1	G	104	LEU
1	G	107	LEU
1	G	108	LEU
1	G	122	GLU
1	G	125	GLU
1	G	154	VAL
1	G	159	VAL
1	G	167	PHE
1	G	174	LEU
1	G	192	LEU
1	G	200	MET
1	G	243	HIS
1	G	248	ILE
1	G	251	TYR
1	G	271	LEU
1	G	275	MET
1	G	278	ILE
1	G	289	ASN
1	G	294	LEU
1	G	313	SER
1	G	319	MET
1	G	372	ARG
1	G	373	GLU
1	G	427	LEU
1	G	454	ASN
1	G	467	TYR
2	H	7	LEU
2	H	13	LEU
2	H	16	LEU
2	H	17	PHE
2	H	22	VAL

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Mol	Chain	Res	Type
2	H	27	LEU
2	H	44	GLU
2	H	62	ARG
2	H	92	SER
2	H	112	VAL
2	H	127	ASN
2	H	129	ARG
2	H	169	GLU
2	H	177	ASP
3	I	4	PHE
3	I	8	TYR
3	I	12	LEU
3	I	16	THR
3	I	20	LEU
3	I	24	ILE
3	I	27	THR
3	I	37	ASP
3	I	38	GLN
3	I	40	MET
3	I	47	ILE
3	I	49	GLU
3	I	62	PHE
3	I	63	ILE
3	I	66	LEU
3	I	73	LEU
3	I	86	LEU
3	I	108	GLU
3	I	127	GLN
3	I	133	LYS
3	I	137	ARG
3	I	163	GLN
3	I	175	LYS
3	I	179	LEU
3	I	182	ARG
3	I	201	VAL
3	I	264	LEU
1	K	50	TRP
1	K	57	ARG
1	K	59	LEU
1	K	64	VAL
1	K	73	LEU
1	K	87	THR

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Mol	Chain	Res	Type
1	K	89	LEU
1	K	90	PHE
1	K	104	LEU
1	K	107	LEU
1	K	108	LEU
1	K	125	GLU
1	K	154	VAL
1	K	159	VAL
1	K	167	PHE
1	K	174	LEU
1	K	192	LEU
1	K	200	MET
1	K	235	TYR
1	K	243	HIS
1	K	251	TYR
1	K	271	LEU
1	K	275	MET
1	K	278	ILE
1	K	289	ASN
1	K	294	LEU
1	K	313	SER
1	K	319	MET
1	K	372	ARG
1	K	373	GLU
1	K	427	LEU
1	K	454	ASN
1	K	466	GLU
1	K	467	TYR
2	L	13	LEU
2	L	16	LEU
2	L	17	PHE
2	L	22	VAL
2	L	27	LEU
2	L	62	ARG
2	L	92	SER
2	L	112	VAL
2	L	127	ASN
2	L	129	ARG
2	L	177	ASP
3	M	8	TYR
3	M	11	LEU
3	M	20	LEU

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Mol	Chain	Res	Type
3	M	24	ILE
3	M	27	THR
3	M	29	LYS
3	M	35	THR
3	M	38	GLN
3	M	40	MET
3	M	44	PHE
3	M	60	LEU
3	M	62	PHE
3	M	68	PHE
3	M	71	LEU
3	M	75	LEU
3	M	130	GLN
3	M	145	ILE
3	M	163	GLN
3	M	175	LYS
3	M	179	LEU
3	M	182	ARG
3	M	201	VAL
3	M	239	GLN
3	M	264	LEU
4	P	21	LEU
4	Q	20	PHE
4	Q	21	LEU
4	Q	27	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (113) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	62	ASN
1	A	82	GLN
1	A	103	GLN
1	A	161	ASN
1	A	178	ASN
1	A	243	HIS
1	A	289	ASN
1	A	374	GLN
1	A	382	ASN
1	A	406	GLN
1	A	414	ASN
1	A	431	HIS

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Mol	Chain	Res	Type
1	A	454	ASN
1	A	460	GLN
2	B	10	ASN
2	B	29	GLN
2	B	36	GLN
2	B	40	ASN
2	B	127	ASN
2	B	193	GLN
3	C	52	ASN
3	C	98	GLN
3	C	105	GLN
3	C	141	ASN
3	C	163	GLN
3	C	231	GLN
3	C	266	GLN
3	C	292	HIS
1	D	16	GLN
1	D	62	ASN
1	D	82	GLN
1	D	103	GLN
1	D	161	ASN
1	D	178	ASN
1	D	243	HIS
1	D	289	ASN
1	D	374	GLN
1	D	382	ASN
1	D	406	GLN
1	D	414	ASN
1	D	431	HIS
1	D	460	GLN
2	E	10	ASN
2	E	29	GLN
2	E	36	GLN
2	E	40	ASN
2	E	127	ASN
2	E	193	GLN
3	F	38	GLN
3	F	42	HIS
3	F	52	ASN
3	F	81	ASN
3	F	163	GLN
3	F	266	GLN

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Mol	Chain	Res	Type
1	G	16	GLN
1	G	62	ASN
1	G	82	GLN
1	G	103	GLN
1	G	156	HIS
1	G	161	ASN
1	G	178	ASN
1	G	289	ASN
1	G	374	GLN
1	G	382	ASN
1	G	406	GLN
1	G	414	ASN
1	G	431	HIS
1	G	454	ASN
2	H	10	ASN
2	H	29	GLN
2	H	36	GLN
2	H	40	ASN
2	H	127	ASN
2	H	193	GLN
3	I	42	HIS
3	I	81	ASN
3	I	105	GLN
3	I	127	GLN
3	I	141	ASN
3	I	163	GLN
3	I	266	GLN
3	I	268	GLN
3	I	276	ASN
3	I	292	HIS
1	K	16	GLN
1	K	62	ASN
1	K	82	GLN
1	K	103	GLN
1	K	161	ASN
1	K	178	ASN
1	K	243	HIS
1	K	289	ASN
1	K	374	GLN
1	K	382	ASN
1	K	406	GLN
1	K	414	ASN

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Mol	Chain	Res	Type
1	K	431	HIS
1	K	454	ASN
1	K	460	GLN
2	L	10	ASN
2	L	29	GLN
2	L	36	GLN
2	L	40	ASN
2	L	71	GLN
2	L	127	ASN
2	L	193	GLN
3	M	38	GLN
3	M	141	ASN
3	M	163	GLN
3	M	266	GLN
3	M	268	GLN
3	M	292	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 44 ligands modelled in this entry, 12 are monoatomic - leaving 32 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	HEM	A	501	1,8,7	24,50,50	2.39	6 (25%)	16,82,82	1.78	4 (25%)
5	HEM	A	502	1,7	24,50,50	2.50	6 (25%)	16,82,82	1.37	1 (6%)
8	PEO	A	505	5,6	1,1,1	0.44	0	0,0,0	0.00	-
9	PO4	A	506	-	4,4,4	0.74	0	6,6,6	0.22	0
10	HEC	B	301	2	24,50,50	2.50	12 (50%)	19,82,82	3.16	9 (47%)
10	HEC	C	401	3	24,50,50	2.67	11 (45%)	19,82,82	3.25	11 (57%)
10	HEC	C	402	3	24,50,50	2.66	11 (45%)	19,82,82	3.07	14 (73%)
11	FC6	C	403	-	12,12,12	2.56	6 (50%)	0,21,21	0.00	-
5	HEM	D	501	1,8,7	24,50,50	2.36	6 (25%)	16,82,82	1.42	2 (12%)
5	HEM	D	502	1,7	24,50,50	2.44	6 (25%)	16,82,82	1.53	2 (12%)
9	PO4	D	505	-	4,4,4	0.70	0	6,6,6	0.23	0
8	PEO	D	506	5,6	1,1,1	0.48	0	0,0,0	0.00	-
10	HEC	E	301	2	24,50,50	2.56	11 (45%)	19,82,82	2.90	9 (47%)
10	HEC	F	401	3	24,50,50	2.71	11 (45%)	19,82,82	3.00	8 (42%)
10	HEC	F	402	3	24,50,50	2.84	11 (45%)	19,82,82	2.75	10 (52%)
11	FC6	F	403	-	12,12,12	2.63	6 (50%)	0,21,21	0.00	-
5	HEM	G	501	1,8,7	24,50,50	2.32	6 (25%)	16,82,82	1.68	4 (25%)
5	HEM	G	502	1,7	24,50,50	2.46	6 (25%)	16,82,82	1.64	4 (25%)
8	PEO	G	505	5,6	1,1,1	0.55	0	0,0,0	0.00	-
9	PO4	G	506	-	4,4,4	0.75	0	6,6,6	0.23	0
10	HEC	H	301	2	24,50,50	2.58	12 (50%)	19,82,82	3.12	8 (42%)
11	FC6	I	401	-	12,12,12	2.65	6 (50%)	0,21,21	0.00	-
10	HEC	I	402	3	24,50,50	2.73	11 (45%)	19,82,82	3.13	12 (63%)
10	HEC	I	403	3	24,50,50	2.62	11 (45%)	19,82,82	3.01	12 (63%)
5	HEM	K	501	1,8,7	24,50,50	2.33	7 (29%)	16,82,82	1.40	1 (6%)
5	HEM	K	502	1,7	24,50,50	2.43	6 (25%)	16,82,82	1.56	3 (18%)
9	PO4	K	506	-	4,4,4	0.89	0	6,6,6	0.26	0
8	PEO	K	507	5,6	1,1,1	0.48	0	0,0,0	0.00	-
10	HEC	L	301	2	24,50,50	2.51	11 (45%)	19,82,82	3.07	10 (52%)
11	FC6	M	401	-	12,12,12	2.58	6 (50%)	0,21,21	0.00	-
10	HEC	M	402	3	24,50,50	2.60	11 (45%)	19,82,82	3.40	11 (57%)
10	HEC	M	403	3	24,50,50	2.66	10 (41%)	19,82,82	3.03	11 (57%)

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
5	HEM	A	501	1,8,7	-	0/6/54/54	0/0/8/8
5	HEM	A	502	1,7	-	0/6/54/54	0/0/8/8
8	PEO	A	505	5,6	-	0/0/0/0	0/0/0/0
9	PO4	A	506	-	-	0/0/0/0	0/0/0/0
10	HEC	B	301	2	-	0/6/54/54	0/0/8/8
10	HEC	C	401	3	-	0/6/54/54	0/0/8/8
10	HEC	C	402	3	-	0/6/54/54	0/0/8/8
11	FC6	C	403	-	-	0/0/30/30	0/0/0/0
5	HEM	D	501	1,8,7	-	0/6/54/54	0/0/8/8
5	HEM	D	502	1,7	-	0/6/54/54	0/0/8/8
9	PO4	D	505	-	-	0/0/0/0	0/0/0/0
8	PEO	D	506	5,6	-	0/0/0/0	0/0/0/0
10	HEC	E	301	2	-	0/6/54/54	0/0/8/8
10	HEC	F	401	3	-	0/6/54/54	0/0/8/8
10	HEC	F	402	3	-	0/6/54/54	0/0/8/8
11	FC6	F	403	-	-	0/0/30/30	0/0/0/0
5	HEM	G	501	1,8,7	-	0/6/54/54	0/0/8/8
5	HEM	G	502	1,7	-	0/6/54/54	0/0/8/8
8	PEO	G	505	5,6	-	0/0/0/0	0/0/0/0
9	PO4	G	506	-	-	0/0/0/0	0/0/0/0
10	HEC	H	301	2	-	0/6/54/54	0/0/8/8
11	FC6	I	401	-	-	0/0/30/30	0/0/0/0
10	HEC	I	402	3	-	0/6/54/54	0/0/8/8
10	HEC	I	403	3	-	0/6/54/54	0/0/8/8
5	HEM	K	501	1,8,7	-	0/6/54/54	0/0/8/8
5	HEM	K	502	1,7	-	0/6/54/54	0/0/8/8
9	PO4	K	506	-	-	0/0/0/0	0/0/0/0
8	PEO	K	507	5,6	-	0/0/0/0	0/0/0/0
10	HEC	L	301	2	-	0/6/54/54	0/0/8/8
11	FC6	M	401	-	-	0/0/30/30	0/0/0/0
10	HEC	M	402	3	-	0/6/54/54	0/0/8/8
10	HEC	M	403	3	-	0/6/54/54	0/0/8/8

All (206) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	502	HEM	C3C-C2C	-5.89	1.32	1.40
5	A	502	HEM	C3B-C2B	-5.78	1.33	1.40
5	G	502	HEM	C3C-C2C	-5.76	1.33	1.40
5	D	502	HEM	C3C-C2C	-5.52	1.33	1.40
5	K	502	HEM	C3C-C2C	-5.46	1.33	1.40
5	A	501	HEM	C3C-C2C	-5.46	1.33	1.40
5	G	502	HEM	C3B-C2B	-5.38	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	501	HEM	C3C-C2C	-5.32	1.33	1.40
5	K	502	HEM	C3B-C2B	-5.29	1.33	1.40
5	K	501	HEM	C3C-C2C	-5.23	1.33	1.40
5	D	502	HEM	C3B-C2B	-5.09	1.33	1.40
5	D	501	HEM	C3C-C2C	-5.07	1.33	1.40
11	F	403	FC6	C24-FE2	-4.41	1.80	1.93
11	I	401	FC6	C22-FE2	-4.38	1.80	1.93
5	A	501	HEM	C3B-C2B	-4.36	1.34	1.40
11	C	403	FC6	C24-FE2	-4.32	1.80	1.93
11	I	401	FC6	C24-FE2	-4.26	1.80	1.93
5	D	501	HEM	C3B-C2B	-4.13	1.35	1.40
11	F	403	FC6	C22-FE2	-4.12	1.81	1.93
5	G	501	HEM	C3B-C2B	-4.09	1.35	1.40
11	M	401	FC6	C11-FE2	-4.00	1.81	1.93
5	K	501	HEM	C3B-C2B	-3.99	1.35	1.40
11	C	403	FC6	C26-FE2	-3.84	1.82	1.93
11	C	403	FC6	C21-FE2	-3.74	1.82	1.93
11	I	401	FC6	C21-FE2	-3.73	1.82	1.93
11	F	403	FC6	C21-FE2	-3.71	1.82	1.93
11	M	401	FC6	C21-FE2	-3.66	1.82	1.93
11	M	401	FC6	C22-FE2	-3.65	1.82	1.93
11	M	401	FC6	C24-FE2	-3.62	1.82	1.93
11	I	401	FC6	C23-FE2	-3.51	1.83	1.93
11	M	401	FC6	C26-FE2	-3.44	1.83	1.93
11	F	403	FC6	C23-FE2	-3.43	1.83	1.93
10	F	401	HEC	C4B-NB	-3.43	1.32	1.36
10	B	301	HEC	C4B-NB	-3.26	1.32	1.36
11	I	401	FC6	C11-FE2	-3.24	1.83	1.93
11	C	403	FC6	C23-FE2	-3.23	1.83	1.93
10	L	301	HEC	C4B-NB	-3.23	1.32	1.36
11	C	403	FC6	C22-FE2	-3.22	1.83	1.93
11	M	401	FC6	C23-FE2	-3.20	1.84	1.93
10	E	301	HEC	C4B-NB	-3.11	1.32	1.36
11	F	403	FC6	C11-FE2	-3.11	1.84	1.93
11	F	403	FC6	C26-FE2	-3.10	1.84	1.93
10	M	403	HEC	C4B-NB	-3.09	1.32	1.36
10	H	301	HEC	C4B-NB	-3.04	1.32	1.36
10	I	402	HEC	C4B-NB	-3.00	1.32	1.36
10	M	402	HEC	C4B-NB	-2.98	1.32	1.36
11	C	403	FC6	C11-FE2	-2.94	1.84	1.93
10	F	402	HEC	C4B-NB	-2.93	1.32	1.36
10	I	403	HEC	C4B-NB	-2.76	1.33	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	I	401	FC6	C26-FE2	-2.76	1.85	1.93
10	C	401	HEC	C4B-NB	-2.72	1.33	1.36
10	C	402	HEC	C4B-NB	-2.70	1.33	1.36
10	B	301	HEC	C1A-NA	-2.42	1.33	1.36
10	H	301	HEC	C1A-NA	-2.03	1.34	1.36
10	F	402	HEC	C3B-C4B	2.02	1.46	1.43
10	C	402	HEC	C3B-C4B	2.04	1.46	1.43
5	K	501	HEM	CAD-C3D	2.04	1.54	1.52
5	G	502	HEM	C4D-ND	2.05	1.39	1.36
10	F	401	HEC	C3B-C4B	2.06	1.46	1.43
10	L	301	HEC	C1C-CHC	2.07	1.45	1.40
5	K	501	HEM	C4D-ND	2.09	1.39	1.36
5	A	502	HEM	C4D-ND	2.09	1.39	1.36
10	L	301	HEC	C3B-C4B	2.09	1.46	1.43
10	I	403	HEC	C3B-C4B	2.09	1.46	1.43
5	D	502	HEM	C4D-ND	2.12	1.39	1.36
10	I	403	HEC	C1C-CHC	2.13	1.45	1.40
10	M	403	HEC	C1C-CHC	2.15	1.45	1.40
10	M	402	HEC	C1C-CHC	2.15	1.45	1.40
5	D	501	HEM	CAD-C3D	2.18	1.55	1.52
10	B	301	HEC	C1C-CHC	2.18	1.46	1.40
10	C	402	HEC	C1C-CHC	2.19	1.46	1.40
10	F	402	HEC	C1C-CHC	2.20	1.46	1.40
10	M	402	HEC	C3B-C4B	2.24	1.47	1.43
5	K	502	HEM	C4D-ND	2.26	1.39	1.36
10	F	401	HEC	C1C-CHC	2.28	1.46	1.40
10	H	301	HEC	C3B-C4B	2.28	1.47	1.43
10	B	301	HEC	C3B-C4B	2.30	1.47	1.43
10	H	301	HEC	C1C-CHC	2.33	1.46	1.40
10	E	301	HEC	C3B-C4B	2.34	1.47	1.43
10	I	402	HEC	C1C-CHC	2.38	1.46	1.40
10	I	402	HEC	C3B-C4B	2.43	1.47	1.43
10	H	301	HEC	C1B-CHB	2.43	1.46	1.40
10	C	401	HEC	C1B-CHB	2.45	1.46	1.40
10	E	301	HEC	C1C-CHC	2.48	1.46	1.40
10	C	401	HEC	C1C-CHC	2.53	1.46	1.40
10	I	402	HEC	C1B-CHB	2.53	1.46	1.40
10	C	402	HEC	C1B-CHB	2.53	1.46	1.40
5	G	501	HEM	C4D-ND	2.54	1.40	1.36
10	L	301	HEC	C1D-CHD	2.58	1.47	1.40
10	E	301	HEC	C1B-CHB	2.62	1.47	1.40
10	B	301	HEC	C4D-CHA	2.63	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	E	301	HEC	C1D-CHD	2.63	1.47	1.40
10	M	403	HEC	C1D-CHD	2.65	1.47	1.40
10	M	402	HEC	C1B-CHB	2.65	1.47	1.40
10	C	401	HEC	C3B-C4B	2.66	1.48	1.43
10	I	403	HEC	C1B-CHB	2.66	1.47	1.40
10	B	301	HEC	C1D-CHD	2.68	1.47	1.40
10	L	301	HEC	C1B-CHB	2.70	1.47	1.40
10	H	301	HEC	C1D-CHD	2.71	1.47	1.40
10	C	402	HEC	C1D-CHD	2.72	1.47	1.40
10	B	301	HEC	C1B-CHB	2.77	1.47	1.40
10	H	301	HEC	C4D-CHA	2.78	1.47	1.40
10	F	401	HEC	C1B-CHB	2.79	1.47	1.40
10	I	403	HEC	C1D-CHD	2.85	1.47	1.40
10	I	402	HEC	C1D-CHD	2.85	1.47	1.40
10	M	403	HEC	C1B-CHB	2.86	1.47	1.40
10	F	402	HEC	C1B-CHB	2.87	1.47	1.40
10	M	402	HEC	C1D-CHD	2.90	1.47	1.40
10	M	402	HEC	C4D-CHA	2.93	1.48	1.40
10	E	301	HEC	C4D-CHA	2.94	1.48	1.40
10	E	301	HEC	C3C-C4C	2.94	1.48	1.43
10	M	402	HEC	C2A-C3A	2.96	1.46	1.37
10	L	301	HEC	C3C-C4C	3.01	1.48	1.43
10	I	402	HEC	C4D-CHA	3.02	1.48	1.40
10	C	401	HEC	C1D-CHD	3.02	1.48	1.40
10	B	301	HEC	C3D-C2D	3.05	1.46	1.37
10	C	401	HEC	C4D-CHA	3.05	1.48	1.40
5	A	501	HEM	C4D-ND	3.07	1.40	1.36
10	C	401	HEC	C2A-C3A	3.07	1.46	1.37
10	I	403	HEC	C4D-CHA	3.08	1.48	1.40
10	L	301	HEC	C4D-CHA	3.10	1.48	1.40
10	H	301	HEC	C3C-C4C	3.10	1.48	1.43
10	F	401	HEC	C4D-CHA	3.13	1.48	1.40
10	B	301	HEC	C3C-C4C	3.14	1.48	1.43
10	M	402	HEC	C3D-C2D	3.14	1.47	1.37
10	M	403	HEC	C4D-CHA	3.15	1.48	1.40
10	I	403	HEC	C3D-C2D	3.15	1.47	1.37
10	C	402	HEC	C3D-C2D	3.15	1.47	1.37
10	B	301	HEC	C2A-C3A	3.16	1.47	1.37
10	F	402	HEC	C1D-CHD	3.19	1.48	1.40
10	I	402	HEC	C2A-C3A	3.21	1.47	1.37
10	M	403	HEC	C2A-C3A	3.22	1.47	1.37
5	A	502	HEM	C3B-CAB	3.23	1.54	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	I	403	HEC	C2A-C3A	3.23	1.47	1.37
10	E	301	HEC	C2A-C3A	3.26	1.47	1.37
10	M	403	HEC	C3D-C2D	3.26	1.47	1.37
10	C	402	HEC	C4D-CHA	3.26	1.48	1.40
10	I	402	HEC	C3D-C2D	3.28	1.47	1.37
10	F	401	HEC	C2A-C3A	3.29	1.47	1.37
10	I	403	HEC	C3C-C4C	3.30	1.49	1.43
10	M	403	HEC	C3C-C4C	3.30	1.49	1.43
10	F	401	HEC	C1D-CHD	3.31	1.49	1.40
10	F	402	HEC	C4D-CHA	3.32	1.49	1.40
10	E	301	HEC	C3D-C2D	3.33	1.47	1.37
10	F	401	HEC	C3D-C2D	3.35	1.47	1.37
10	L	301	HEC	C3D-C2D	3.36	1.47	1.37
10	C	402	HEC	C2A-C3A	3.38	1.47	1.37
10	H	301	HEC	C3D-C2D	3.38	1.47	1.37
5	G	502	HEM	C3B-CAB	3.38	1.55	1.47
10	H	301	HEC	C2A-C3A	3.38	1.47	1.37
5	A	502	HEM	C3C-CAC	3.38	1.54	1.47
10	F	402	HEC	C3D-C2D	3.39	1.47	1.37
10	C	401	HEC	C3D-C2D	3.40	1.47	1.37
10	F	402	HEC	C2A-C3A	3.40	1.47	1.37
10	L	301	HEC	C2A-C3A	3.43	1.47	1.37
5	A	501	HEM	C3C-CAC	3.45	1.54	1.47
10	C	402	HEC	C3C-C4C	3.46	1.49	1.43
5	K	502	HEM	C3B-CAB	3.50	1.55	1.47
5	D	502	HEM	C3B-CAB	3.57	1.55	1.47
5	G	502	HEM	C3C-CAC	3.57	1.55	1.47
10	M	402	HEC	C3C-C4C	3.58	1.49	1.43
5	K	501	HEM	C3C-CAC	3.59	1.55	1.47
5	K	502	HEM	C3C-CAC	3.63	1.55	1.47
10	I	402	HEC	C3C-C4C	3.64	1.49	1.43
5	G	501	HEM	C3B-CAB	3.65	1.55	1.47
5	G	501	HEM	C3C-CAC	3.67	1.55	1.47
5	A	501	HEM	C3B-CAB	3.68	1.55	1.47
5	D	502	HEM	C3C-CAC	3.68	1.55	1.47
5	D	501	HEM	C3B-CAB	3.71	1.55	1.47
10	F	402	HEC	C3C-C4C	3.76	1.50	1.43
5	K	501	HEM	C3B-CAB	3.76	1.55	1.47
5	D	501	HEM	C3C-CAC	3.86	1.55	1.47
10	F	401	HEC	C3C-C4C	4.17	1.50	1.43
10	C	401	HEC	C3C-C4C	4.57	1.51	1.43
10	L	301	HEC	C3B-C2B	5.12	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	502	HEM	C3D-C2D	5.25	1.53	1.37
5	G	501	HEM	C3D-C2D	5.25	1.53	1.37
10	H	301	HEC	C3B-C2B	5.30	1.46	1.40
5	K	502	HEM	C3D-C2D	5.31	1.53	1.37
10	B	301	HEC	C3B-C2B	5.31	1.46	1.40
5	D	502	HEM	C3D-C2D	5.33	1.53	1.37
5	A	501	HEM	C3D-C2D	5.33	1.53	1.37
5	G	502	HEM	C3D-C2D	5.46	1.53	1.37
5	K	501	HEM	C3D-C2D	5.49	1.54	1.37
5	D	501	HEM	C3D-C2D	5.58	1.54	1.37
10	E	301	HEC	C3B-C2B	5.67	1.46	1.40
10	M	402	HEC	C3B-C2B	5.68	1.46	1.40
10	C	401	HEC	C3B-C2B	5.84	1.46	1.40
10	F	401	HEC	C3B-C2B	5.99	1.46	1.40
10	I	403	HEC	C3B-C2B	6.07	1.47	1.40
10	B	301	HEC	C3C-C2C	6.28	1.47	1.40
10	C	401	HEC	C3C-C2C	6.33	1.47	1.40
10	I	402	HEC	C3B-C2B	6.34	1.47	1.40
10	M	403	HEC	C3B-C2B	6.36	1.47	1.40
10	C	402	HEC	C3B-C2B	6.43	1.47	1.40
10	L	301	HEC	C3C-C2C	6.48	1.47	1.40
10	C	402	HEC	C3C-C2C	6.52	1.47	1.40
10	M	402	HEC	C3C-C2C	6.60	1.47	1.40
10	E	301	HEC	C3C-C2C	6.68	1.47	1.40
10	F	401	HEC	C3C-C2C	6.73	1.47	1.40
10	M	403	HEC	C3C-C2C	6.81	1.47	1.40
10	I	403	HEC	C3C-C2C	6.83	1.47	1.40
10	I	402	HEC	C3C-C2C	6.98	1.48	1.40
10	H	301	HEC	C3C-C2C	7.00	1.48	1.40
10	F	402	HEC	C3C-C2C	7.21	1.48	1.40
10	F	402	HEC	C3B-C2B	7.22	1.48	1.40

All (146) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	B	301	HEC	CBB-CAB-C3B	-7.64	110.64	127.34
10	E	301	HEC	CBB-CAB-C3B	-7.38	111.20	127.34
10	B	301	HEC	CBA-CAA-C2A	-7.34	99.59	112.47
10	L	301	HEC	CBB-CAB-C3B	-7.28	111.42	127.34
10	M	402	HEC	CAA-CBA-CGA	-7.21	98.75	112.78
10	H	301	HEC	CBB-CAB-C3B	-7.20	111.59	127.34
10	H	301	HEC	CBA-CAA-C2A	-6.40	101.24	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	M	402	HEC	CBB-CAB-C3B	-6.33	113.51	127.34
10	M	402	HEC	CBD-CAD-C3D	-6.25	101.50	112.49
10	C	401	HEC	CBD-CAD-C3D	-5.88	102.15	112.49
10	I	402	HEC	CAA-CBA-CGA	-5.77	101.56	112.78
10	I	403	HEC	CAD-CBD-CGD	-5.66	101.77	112.78
10	L	301	HEC	CBA-CAA-C2A	-5.62	102.61	112.47
10	C	401	HEC	CBB-CAB-C3B	-5.34	115.66	127.34
10	F	401	HEC	CBB-CAB-C3B	-5.34	115.66	127.34
10	C	401	HEC	CAA-CBA-CGA	-5.30	102.47	112.78
10	E	301	HEC	CBA-CAA-C2A	-5.27	103.23	112.47
10	I	402	HEC	CBB-CAB-C3B	-5.26	115.83	127.34
10	F	401	HEC	CBD-CAD-C3D	-5.25	103.26	112.49
10	C	401	HEC	CBC-CAC-C3C	-5.11	116.16	127.34
10	F	402	HEC	C4B-C3B-C2B	-5.07	100.21	106.19
10	F	401	HEC	CAA-CBA-CGA	-5.02	103.01	112.78
10	C	402	HEC	CBB-CAB-C3B	-4.88	116.68	127.34
10	M	403	HEC	CAD-CBD-CGD	-4.86	103.32	112.78
10	C	402	HEC	C4B-C3B-C2B	-4.80	100.53	106.19
10	I	402	HEC	CBD-CAD-C3D	-4.76	104.12	112.49
10	C	402	HEC	CAD-CBD-CGD	-4.75	103.53	112.78
10	M	403	HEC	CBB-CAB-C3B	-4.72	117.01	127.34
10	I	403	HEC	C4B-C3B-C2B	-4.72	100.62	106.19
10	F	402	HEC	CBB-CAB-C3B	-4.60	117.28	127.34
10	I	403	HEC	CBB-CAB-C3B	-4.54	117.41	127.34
10	M	403	HEC	C4B-C3B-C2B	-4.50	100.89	106.19
10	F	401	HEC	C4B-C3B-C2B	-4.45	100.94	106.19
10	C	401	HEC	C4C-C3C-C2C	-4.42	100.97	106.19
10	L	301	HEC	CBC-CAC-C3C	-4.12	118.33	127.34
10	M	403	HEC	CAA-CBA-CGA	-4.06	104.88	112.78
10	H	301	HEC	CBC-CAC-C3C	-4.05	118.49	127.34
10	C	401	HEC	C4B-C3B-C2B	-4.05	101.42	106.19
10	C	402	HEC	CBA-CAA-C2A	-4.04	105.39	112.47
10	E	301	HEC	CBC-CAC-C3C	-4.01	118.57	127.34
10	I	402	HEC	C4B-C3B-C2B	-3.83	101.68	106.19
10	M	403	HEC	CBC-CAC-C3C	-3.82	118.99	127.34
10	B	301	HEC	CBC-CAC-C3C	-3.79	119.05	127.34
10	I	402	HEC	C4C-C3C-C2C	-3.76	101.75	106.19
10	M	402	HEC	C4B-C3B-C2B	-3.75	101.77	106.19
10	M	402	HEC	CBC-CAC-C3C	-3.69	119.27	127.34
5	A	501	HEM	CAD-CBD-CGD	-3.65	105.69	112.78
10	C	402	HEC	CAA-CBA-CGA	-3.55	105.87	112.78
5	G	502	HEM	CBA-CAA-C2A	-3.35	106.60	112.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	G	501	HEM	CAA-CBA-CGA	-3.26	106.43	112.78
5	G	501	HEM	CAD-CBD-CGD	-3.26	106.44	112.78
5	D	501	HEM	CAD-CBD-CGD	-3.26	106.45	112.78
10	I	403	HEC	CBA-CAA-C2A	-3.21	106.84	112.47
10	L	301	HEC	C4B-C3B-C2B	-3.20	102.42	106.19
5	K	501	HEM	CAD-CBD-CGD	-3.19	106.58	112.78
10	C	402	HEC	CBC-CAC-C3C	-3.16	120.44	127.34
5	D	502	HEM	CBA-CAA-C2A	-3.16	106.94	112.49
10	H	301	HEC	C4B-C3B-C2B	-3.10	102.53	106.19
5	G	501	HEM	CBA-CAA-C2A	-3.10	107.05	112.49
10	I	402	HEC	CBC-CAC-C3C	-3.06	120.65	127.34
5	A	502	HEM	CBA-CAA-C2A	-3.04	107.14	112.49
10	E	301	HEC	C4B-C3B-C2B	-3.04	102.61	106.19
10	F	401	HEC	C4C-C3C-C2C	-3.02	102.63	106.19
5	D	502	HEM	CBD-CAD-C3D	-2.89	107.39	112.47
10	C	402	HEC	C4C-C3C-C2C	-2.88	102.79	106.19
5	K	502	HEM	CBD-CAD-C3D	-2.84	107.48	112.47
10	M	403	HEC	C4C-C3C-C2C	-2.82	102.86	106.19
10	B	301	HEC	C4B-C3B-C2B	-2.81	102.88	106.19
10	I	403	HEC	CAA-CBA-CGA	-2.78	107.38	112.78
10	F	401	HEC	CBC-CAC-C3C	-2.76	121.31	127.34
10	I	403	HEC	CBC-CAC-C3C	-2.73	121.37	127.34
10	I	403	HEC	C4C-C3C-C2C	-2.69	103.02	106.19
10	M	402	HEC	C4C-C3C-C2C	-2.68	103.04	106.19
10	L	301	HEC	C4C-C3C-C2C	-2.67	103.04	106.19
5	A	501	HEM	CAA-CBA-CGA	-2.66	107.61	112.78
10	M	403	HEC	CBA-CAA-C2A	-2.62	107.87	112.47
10	F	402	HEC	CBC-CAC-C3C	-2.58	121.69	127.34
10	F	402	HEC	CBA-CAA-C2A	-2.57	107.96	112.47
10	E	301	HEC	C4C-C3C-C2C	-2.56	103.17	106.19
10	F	402	HEC	CAD-CBD-CGD	-2.56	107.79	112.78
10	F	402	HEC	C4C-C3C-C2C	-2.56	103.18	106.19
5	K	502	HEM	CBA-CAA-C2A	-2.55	108.01	112.49
10	C	401	HEC	CAD-CBD-CGD	-2.50	107.92	112.78
10	I	402	HEC	CAD-CBD-CGD	-2.50	107.92	112.78
10	M	402	HEC	CAD-CBD-CGD	-2.50	107.92	112.78
5	G	502	HEM	CMA-C3A-C4A	-2.48	124.09	128.31
10	H	301	HEC	C4C-C3C-C2C	-2.45	103.30	106.19
5	G	502	HEM	CBD-CAD-C3D	-2.42	108.23	112.47
5	K	502	HEM	CMA-C3A-C4A	-2.39	124.25	128.31
10	F	402	HEC	CAA-CBA-CGA	-2.37	108.18	112.78
10	B	301	HEC	C4C-C3C-C2C	-2.36	103.41	106.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	501	HEM	C3C-CAC-CBC	-2.35	121.68	126.40
10	C	402	HEC	CBD-CAD-C3D	-2.31	108.44	112.49
5	D	501	HEM	CBA-CAA-C2A	-2.12	108.76	112.49
10	I	402	HEC	CMC-C2C-C1C	-2.05	124.82	128.31
10	L	301	HEC	CBD-CAD-C3D	-2.05	108.89	112.49
5	G	502	HEM	C3C-CAC-CBC	-2.04	122.30	126.40
10	I	403	HEC	CBD-CAD-C3D	-2.03	108.93	112.49
10	C	402	HEC	C3C-C4C-NC	2.01	114.74	110.94
10	I	403	HEC	CMA-C3A-C2A	2.02	129.47	125.24
10	I	403	HEC	CMB-C2B-C3B	2.03	128.03	125.67
10	C	401	HEC	CMA-C3A-C2A	2.07	129.57	125.24
10	M	402	HEC	CMA-C3A-C2A	2.08	129.59	125.24
10	E	301	HEC	CMA-C3A-C2A	2.12	129.67	125.24
5	G	501	HEM	CMB-C2B-C3B	2.12	129.24	125.09
10	B	301	HEC	CMB-C2B-C3B	2.14	128.15	125.67
10	C	402	HEC	CMD-C2D-C3D	2.17	129.78	125.24
10	M	403	HEC	CMD-C2D-C3D	2.19	129.82	125.24
10	L	301	HEC	CMB-C2B-C3B	2.20	128.22	125.67
10	F	402	HEC	CMB-C2B-C3B	2.27	128.29	125.67
10	C	402	HEC	CMA-C3A-C2A	2.37	130.20	125.24
10	B	301	HEC	CMA-C3A-C2A	2.39	130.23	125.24
10	E	301	HEC	CMB-C2B-C3B	2.41	128.46	125.67
10	M	402	HEC	CMB-C2B-C3B	2.42	128.47	125.67
10	I	402	HEC	CMA-C3A-C2A	2.44	130.34	125.24
10	M	402	HEC	C3B-C4B-NB	2.59	115.84	110.94
10	C	401	HEC	C3B-C4B-NB	2.60	115.86	110.94
5	A	501	HEM	CMB-C2B-C3B	2.62	130.21	125.09
10	I	402	HEC	C3B-C4B-NB	2.62	115.89	110.94
10	H	301	HEC	CMA-C3A-C2A	2.72	130.93	125.24
10	L	301	HEC	CMA-C3A-C2A	2.77	131.03	125.24
10	M	403	HEC	C3B-C4B-NB	2.78	116.19	110.94
10	C	401	HEC	CMC-C2C-C3C	2.85	128.97	125.67
10	I	402	HEC	CMB-C2B-C3B	2.88	129.00	125.67
10	C	402	HEC	CMB-C2B-C3B	2.92	129.06	125.67
10	M	403	HEC	CMB-C2B-C3B	2.92	129.06	125.67
10	E	301	HEC	C3B-C4B-NB	2.97	116.55	110.94
10	F	401	HEC	C3B-C4B-NB	3.04	116.69	110.94
10	C	402	HEC	C3B-C4B-NB	3.11	116.83	110.94
10	F	402	HEC	C3B-C4B-NB	3.12	116.83	110.94
10	I	403	HEC	C3B-C4B-NB	3.15	116.90	110.94
10	H	301	HEC	C3B-C4B-NB	3.20	116.98	110.94
10	B	301	HEC	C3B-C4B-NB	3.26	117.10	110.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	L	301	HEC	C3B-C4B-NB	3.27	117.11	110.94
10	C	401	HEC	CMB-C2B-C3B	3.47	129.69	125.67
10	B	301	HEC	CMC-C2C-C3C	3.71	129.97	125.67
10	E	301	HEC	CMC-C2C-C3C	3.81	130.09	125.67
10	M	402	HEC	CMC-C2C-C3C	4.64	131.05	125.67
10	H	301	HEC	CMC-C2C-C3C	4.64	131.05	125.67
10	L	301	HEC	CMC-C2C-C3C	4.73	131.16	125.67
10	C	402	HEC	CMC-C2C-C3C	4.74	131.17	125.67
10	I	402	HEC	CMC-C2C-C3C	4.93	131.38	125.67
10	M	403	HEC	CMC-C2C-C3C	5.29	131.81	125.67
10	F	401	HEC	CMC-C2C-C3C	5.37	131.89	125.67
10	I	403	HEC	CMC-C2C-C3C	5.60	132.17	125.67
10	F	402	HEC	CMC-C2C-C3C	6.06	132.70	125.67

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

28 monomers are involved in 129 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	501	HEM	3	0
5	A	502	HEM	9	0
9	A	506	PO4	1	0
10	B	301	HEC	5	0
10	C	401	HEC	8	0
10	C	402	HEC	3	0
11	C	403	FC6	2	0
5	D	501	HEM	5	0
5	D	502	HEM	8	0
9	D	505	PO4	1	0
10	E	301	HEC	6	0
10	F	401	HEC	7	0
10	F	402	HEC	3	0
11	F	403	FC6	2	0
5	G	501	HEM	5	0
5	G	502	HEM	8	0
9	G	506	PO4	1	0
10	H	301	HEC	6	0
11	I	401	FC6	1	0
10	I	402	HEC	8	0
10	I	403	HEC	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	K	501	HEM	5	0
5	K	502	HEM	8	0
9	K	506	PO4	4	0
10	L	301	HEC	4	0
11	M	401	FC6	2	0
10	M	402	HEC	9	0
10	M	403	HEC	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	466/474 (98%)	-0.75	6 (1%) 79 67	45, 76, 129, 206	0
1	D	463/474 (97%)	-0.25	20 (4%) 39 25	76, 153, 234, 310	0
1	G	465/474 (98%)	-0.68	3 (0%) 90 84	55, 90, 142, 254	0
1	K	465/474 (98%)	-0.33	14 (3%) 54 39	61, 145, 226, 280	0
2	B	197/203 (97%)	-0.77	2 (1%) 84 75	42, 70, 126, 169	0
2	E	197/203 (97%)	-0.19	7 (3%) 46 31	68, 138, 213, 279	0
2	H	197/203 (97%)	-0.71	1 (0%) 91 87	54, 83, 146, 202	0
2	L	197/203 (97%)	-0.47	6 (3%) 54 39	52, 110, 215, 322	0
3	C	303/311 (97%)	-0.63	2 (0%) 89 83	41, 83, 138, 192	0
3	F	303/311 (97%)	0.18	23 (7%) 17 9	72, 173, 260, 419	0
3	I	303/311 (97%)	-0.43	7 (2%) 64 49	52, 106, 166, 215	0
3	M	303/311 (97%)	-0.31	15 (4%) 32 19	43, 85, 243, 322	0
4	N	29/36 (80%)	-0.20	2 (6%) 20 11	65, 92, 167, 174	0
4	O	29/36 (80%)	0.86	7 (24%) 1 1	148, 172, 249, 263	0
4	P	29/36 (80%)	-0.12	1 (3%) 49 34	91, 109, 173, 191	0
4	Q	29/36 (80%)	0.47	3 (10%) 9 5	119, 142, 186, 199	0
All	All	3975/4096 (97%)	-0.42	119 (2%) 54 39	41, 107, 219, 419	0

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	466	GLU	9.3
2	E	201	ASN	9.1
2	E	44	GLU	7.7
3	F	3	THR	7.7
3	M	50	TYR	7.3

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Mol	Chain	Res	Type	RSRZ
2	E	202	LYS	7.0
1	K	299	HIS	6.4
1	D	299	HIS	6.2
2	E	37	ASP	5.7
3	F	2	SER	5.1
2	H	202	LYS	5.0
1	D	465	ALA	4.7
1	D	153	LYS	4.6
1	G	8	ALA	4.6
4	O	26	TYR	4.5
1	D	374	GLN	4.0
3	F	90	GLU	4.0
1	D	86	GLN	3.9
1	K	150	ALA	3.9
1	K	153	LYS	3.9
4	O	23	GLY	3.8
3	F	35	THR	3.8
3	F	163	GLN	3.6
1	D	296	GLY	3.6
2	L	202	LYS	3.6
3	M	26	ALA	3.5
3	F	40	MET	3.5
1	A	5	THR	3.5
4	Q	29	TRP	3.4
3	F	34	GLY	3.4
3	F	38	GLN	3.4
3	M	35	THR	3.4
3	F	46	GLY	3.3
1	D	373	GLU	3.3
4	O	1	MET	3.3
4	N	26	TYR	3.2
3	F	48	GLU	3.2
4	O	29	TRP	3.2
1	D	8	ALA	3.2
1	D	302	ARG	3.1
1	G	7	THR	3.1
4	O	27	PHE	3.1
3	M	43	ALA	3.1
3	F	130	GLN	3.1
3	M	37	ASP	3.0
2	B	202	LYS	3.0
1	K	467	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
3	I	42	HIS	3.0
1	K	6	SER	3.0
3	M	34	GLY	2.9
3	M	25	PHE	2.9
4	N	29	TRP	2.8
1	K	302	ARG	2.8
4	P	26	TYR	2.8
1	K	468	ASP	2.8
3	F	31	GLU	2.8
1	K	156	HIS	2.8
3	F	42	HIS	2.8
4	Q	26	TYR	2.8
3	I	35	THR	2.8
1	D	231	GLU	2.8
3	F	129	PRO	2.7
1	K	96	ALA	2.7
3	F	119	ALA	2.7
1	K	466	GLU	2.6
2	E	7	LEU	2.6
1	A	373	GLU	2.6
3	F	36	THR	2.6
3	C	29	LYS	2.6
3	M	48	GLU	2.6
3	F	45	ASP	2.6
1	A	155	LYS	2.5
2	E	170	GLU	2.5
1	D	155	LYS	2.5
3	M	51	ASP	2.5
3	M	36	THR	2.5
3	I	3	THR	2.4
3	M	82	TRP	2.4
3	C	30	GLY	2.4
1	K	461	ALA	2.4
3	M	85	VAL	2.4
3	F	4	PHE	2.4
1	D	150	ALA	2.4
3	M	56	ARG	2.4
1	D	468	ASP	2.4
2	E	13	LEU	2.3
3	M	68	PHE	2.3
4	Q	1	MET	2.3
1	K	192	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
2	L	9	LYS	2.3
1	D	232	ARG	2.3
1	A	463	LYS	2.3
4	O	5	ASN	2.2
3	F	283	GLN	2.2
3	F	22	TRP	2.2
2	L	10	ASN	2.2
3	F	105	GLN	2.2
3	I	29	LYS	2.2
3	F	33	ALA	2.2
3	I	36	THR	2.2
1	D	384	HIS	2.2
3	I	90	GLU	2.2
1	G	467	TYR	2.2
1	A	7	THR	2.2
2	L	35	PHE	2.1
1	D	453	TYR	2.1
1	K	7	THR	2.1
3	M	3	THR	2.1
1	D	463	LYS	2.1
2	L	17	PHE	2.1
3	F	94	THR	2.1
1	D	92	PRO	2.1
1	K	373	GLU	2.0
3	I	163	GLN	2.0
1	D	186	ALA	2.0
4	O	22	ALA	2.0
2	B	44	GLU	2.0
2	L	44	GLU	2.0
1	A	6	SER	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
11	FC6	F	403	13/13	0.78	0.35	4.50	53,61,87,101	13
11	FC6	I	401	13/13	0.91	0.25	1.78	78,94,143,158	13
10	HEC	C	402	43/43	0.94	0.18	1.76	36,54,72,160	0
10	HEC	B	301	43/43	0.96	0.17	1.70	39,55,69,119	0
5	HEM	K	501	43/43	0.96	0.22	1.24	119,135,151,154	0
10	HEC	I	403	43/43	0.97	0.17	0.87	50,61,69,85	0
10	HEC	H	301	43/43	0.98	0.15	0.78	42,53,70,79	0
10	HEC	F	401	43/43	0.96	0.21	0.74	85,103,116,121	0
11	FC6	C	403	13/13	0.98	0.15	0.70	60,75,98,101	13
8	PEO	A	505	2/2	0.97	0.16	0.65	74,74,74,74	0
10	HEC	M	403	43/43	0.98	0.14	0.64	35,51,64,84	0
10	HEC	M	402	43/43	0.98	0.14	0.64	33,42,54,63	0
10	HEC	L	301	43/43	0.98	0.14	0.60	49,65,78,78	0
11	FC6	M	401	13/13	0.98	0.14	0.58	43,60,98,98	13
10	HEC	C	401	43/43	0.98	0.15	0.52	44,57,66,73	0
10	HEC	F	402	43/43	0.96	0.20	0.42	117,134,147,154	0
10	HEC	I	402	43/43	0.98	0.14	0.40	38,54,77,91	0
10	HEC	E	301	43/43	0.98	0.14	0.21	62,73,96,102	0
5	HEM	K	502	43/43	0.98	0.16	0.17	95,108,128,130	0
5	HEM	D	501	43/43	0.98	0.15	0.13	93,119,136,143	0
5	HEM	A	502	43/43	0.98	0.13	0.04	41,54,79,83	0
7	CA	D	504	1/1	0.89	0.21	0.01	151,151,151,151	0
5	HEM	D	502	43/43	0.98	0.15	-0.01	89,110,124,130	0
5	HEM	G	502	43/43	0.98	0.13	-0.23	54,66,77,86	0
9	PO4	D	505	5/5	0.72	0.24	-0.31	180,183,183,185	0
5	HEM	A	501	43/43	0.99	0.12	-0.36	45,63,72,76	0
5	HEM	G	501	43/43	0.99	0.11	-0.97	57,72,84,93	0
7	CA	D	507	1/1	0.98	0.10	-1.05	96,96,96,96	0
7	CA	K	505	1/1	0.95	0.12	-1.06	136,136,136,136	0
9	PO4	A	506	5/5	0.93	0.14	-1.09	60,68,75,88	0
9	PO4	K	506	5/5	0.78	0.16	-1.18	138,141,143,150	0
7	CA	G	507	1/1	0.98	0.09	-1.35	72,72,72,72	0
7	CA	A	504	1/1	0.82	0.09	-1.37	99,99,99,99	0
7	CA	G	504	1/1	0.95	0.08	-1.47	87,87,87,87	0
9	PO4	G	506	5/5	0.91	0.12	-1.65	130,132,139,152	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
8	PEO	K	507	2/2	0.98	0.12	-1.70	131,131,131,131	0
8	PEO	D	506	2/2	0.99	0.11	-1.90	145,145,145,147	0
8	PEO	G	505	2/2	0.99	0.10	-3.08	80,80,80,83	0
7	CA	K	504	1/1	0.96	0.05	-3.60	95,95,95,95	0
6	CU	G	503	1/1	0.98	0.03	-	74,74,74,74	0
7	CA	A	507	1/1	0.98	0.25	-	84,84,84,84	0
6	CU	D	503	1/1	0.94	0.06	-	118,118,118,118	0
6	CU	A	503	1/1	0.94	0.34	-	133,133,133,133	0
6	CU	K	503	1/1	0.91	0.10	-	133,133,133,133	0

6.5 Other polymers (i)

There are no such residues in this entry.