



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:42 AM GMT

PDB ID : 3MK7
Title : The structure of CBB3 cytochrome oxidase
Authors : Buschmann, S.; Warkentin, E.; Michel, H.; Ermler, U.
Deposited on : 2010-04-14
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 ⓘ symbol.

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

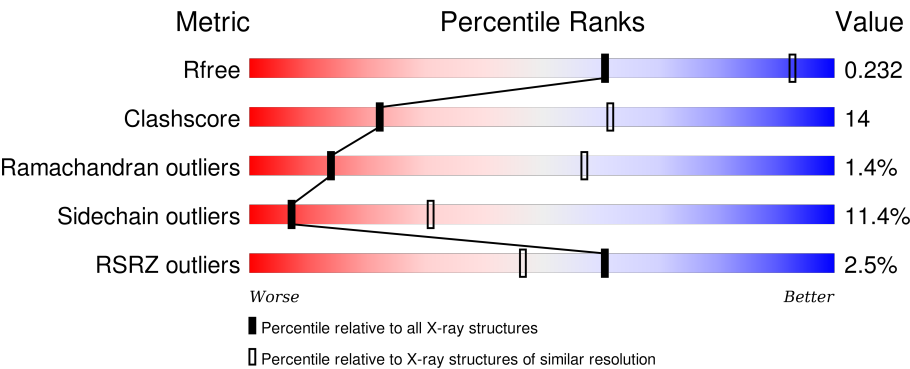
MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	474	<div><div>%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>64%30% . .</div></div>
1	D	474	<div><div>4%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>64%29% . .</div></div>
1	G	474	<div><div>%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>62%32%5% .</div></div>
1	K	474	<div><div>3%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>66%28% . .</div></div>
2	B	203	<div><div></div><div><div></div><div></div><div></div><div></div><div></div></div><div>68%25% . .</div></div>

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Mol	Chain	Length	Quality of chain
2	E	203	
2	H	203	
2	L	203	
3	C	311	
3	F	311	
3	I	311	
3	M	311	
4	U	30	
4	X	30	
4	Y	30	
4	Z	30	

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	C	323	-	-	X	-
11	FC6	F	323	-	-	X	X
11	FC6	I	323	-	-	X	X
9	PO4	G	506	-	-	-	X

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 31690 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 Cytochrome c oxidase, cbb3-type, subunit N.

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 Cytochrome c oxidase, cbb3-type, subunit O.

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 Cytochrome c oxidase, cbb3-type, subunit P.

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			

- | Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|--------------|---------|---------|---------|---------|---------|-------|
| 4 | U | 30 | Total
150 | C
90 | N
30 | O
30 | 0 | 0 | 0 |
| 4 | X | 30 | Total
150 | C
90 | N
30 | O
30 | 0 | 0 | 0 |
| 4 | Y | 30 | Total
150 | C
90 | N
30 | O
30 | 0 | 0 | 0 |
| 4 | Z | 30 | Total
150 | C
90 | N
30 | O
30 | 0 | 0 | 0 |

-
- Chemical structure of HEM (heme) showing a central iron atom coordinated by four nitrogen atoms in a porphyrin-like ring, with various side chains and a central heme group.

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

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

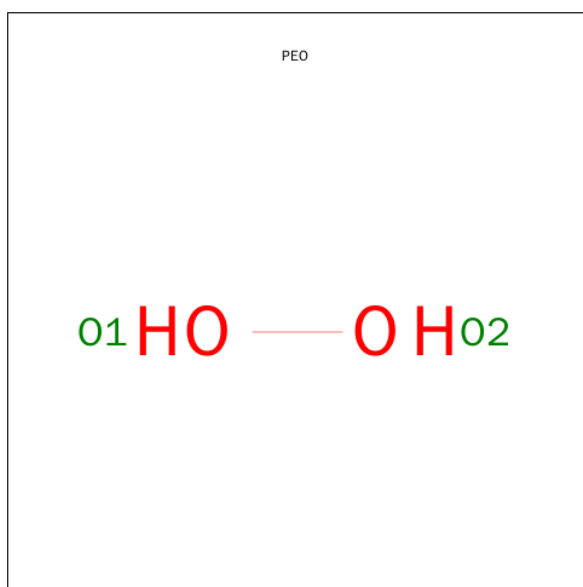
- Molecule 6 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

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

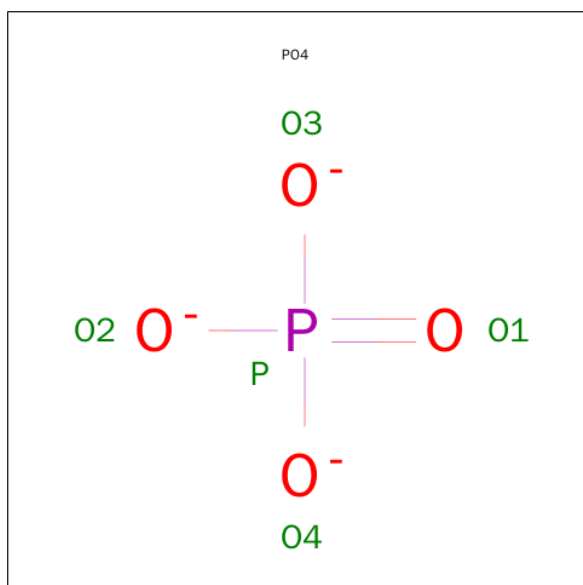
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	G	2	Total	Ca		
			2	2	0	0
7	D	1	Total	Ca		
			1	1	0	0
7	K	2	Total	Ca		
			2	2	0	0
7	E	1	Total	Ca		
			1	1	0	0
7	B	1	Total	Ca		
			1	1	0	0
7	A	1	Total	Ca		
			1	1	0	0

- Molecule 8 is HYDROGEN PEROXIDE (three-letter code: PEO) (formula: H₂O₂).



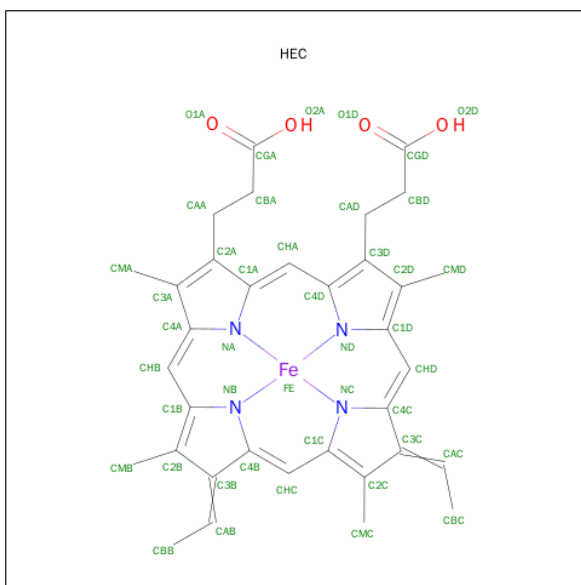
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total O 2 2	0	0
8	D	1	Total O 2 2	0	0
8	G	1	Total O 2 2	0	0
8	K	1	Total O 2 2	0	0

- Molecule 9 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

- Molecule 10 is HEME C (three-letter code: HEC) (formula: $\text{C}_{34}\text{H}_{34}\text{FeN}_4\text{O}_4$).



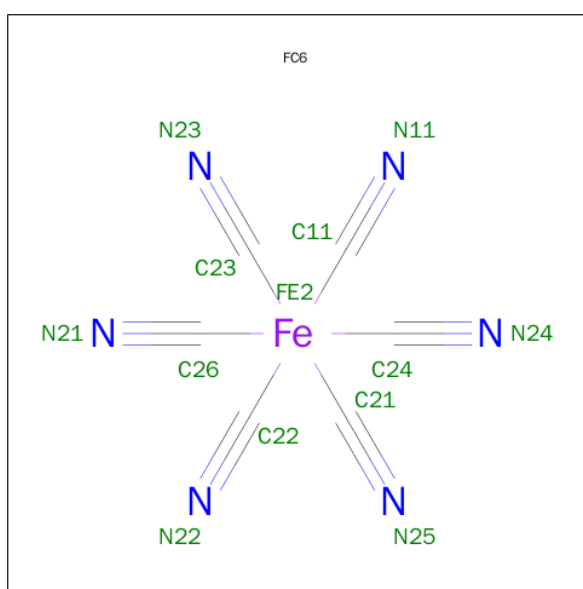
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
10	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
10	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
10	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
10	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
10	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
10	H	1	Total 43	C 34	Fe 1	N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

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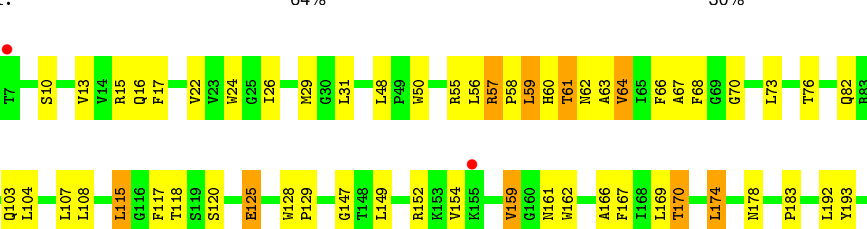
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	I	1	Total	C	Fe	N	O	
			43	34	1	4	4	
10	L	1	Total	C	Fe	N	O	
			43	34	1	4	4	
10	M	1	Total	C	Fe	N	O	
			43	34	1	4	4	
10	M	1	Total	C	Fe	N	O	
			43	34	1	4	4	

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



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

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 ($\text{RSRZ} > 2$). 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.

- Chain A: 

bits

0.64 0.30

0% 100%

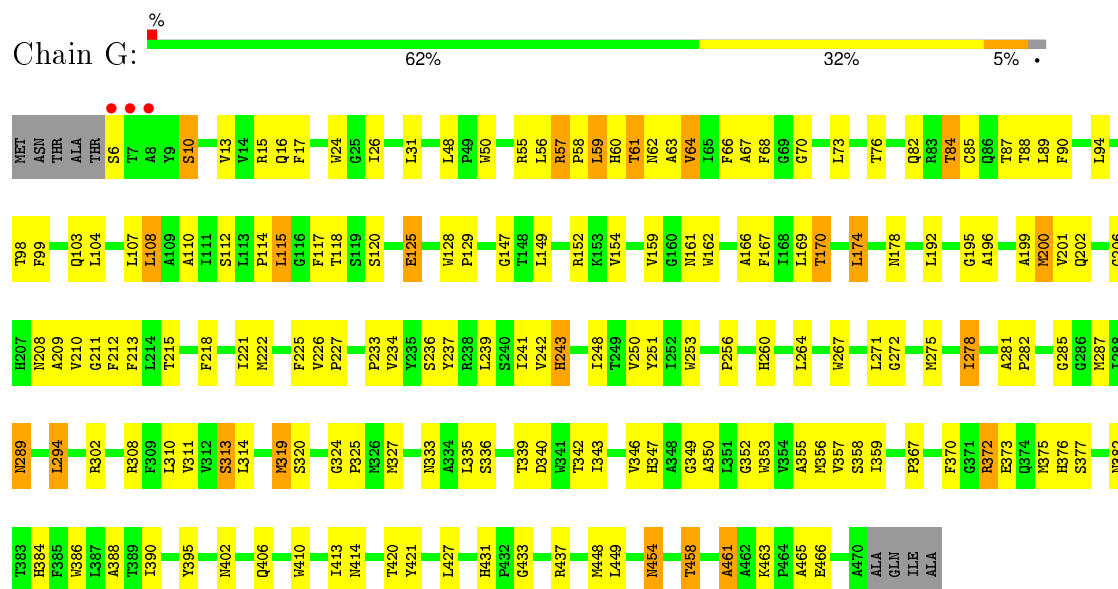
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68 69 70 71 72 73 74 75 76 77 78 79 80 81 82 83 84 85 86 87 88 89 90 91 92 93 94 95 96 97 98 99 100 101 102 103 104 105 106 107 108 109 110 111 112 113 114 115 116 117 118 119 120 121 122 123 124 125 126 127 128 129 130 131 132 133 134 135 136 137 138 139 140 141 142 143 144 145 146 147 148 149 150 151 152 153 154 155 156 157 158 159 160 161 162 163 164 165 166 167 168 169 170 171 172 173 174 175 176 177 178 179 180 181 182 183 184 185 186 187 188 189 190 191 192 193 194 195 196 197 198 199 200

Met ASN THR TIS S6 T7 S10 V13 V14 R15 Q16 F17 V22 V23 Q24 Q25 T26 T27 W28 W29 L31 L48 P49 H50 R55 L56 R57 R58 P59 L59 H60 H61 H62 H63 F66 A67 F68 G69 G70 L73 T76 T77 Q82 R83 R84 C85 T87 T88 T89 T90 L94 T98 P99 Q103 L104 L107 L108 L115 G116 F117 T118 S119 S120 E126 W128 P129 G147 T148 R139 L149 R152 R153 V154 R155 V159 G160 H161 W162 A166 F167 T168 L169 T170 L174 W178 P183 L192 Y193 A196 M200 V201 Q202 Q203 T204

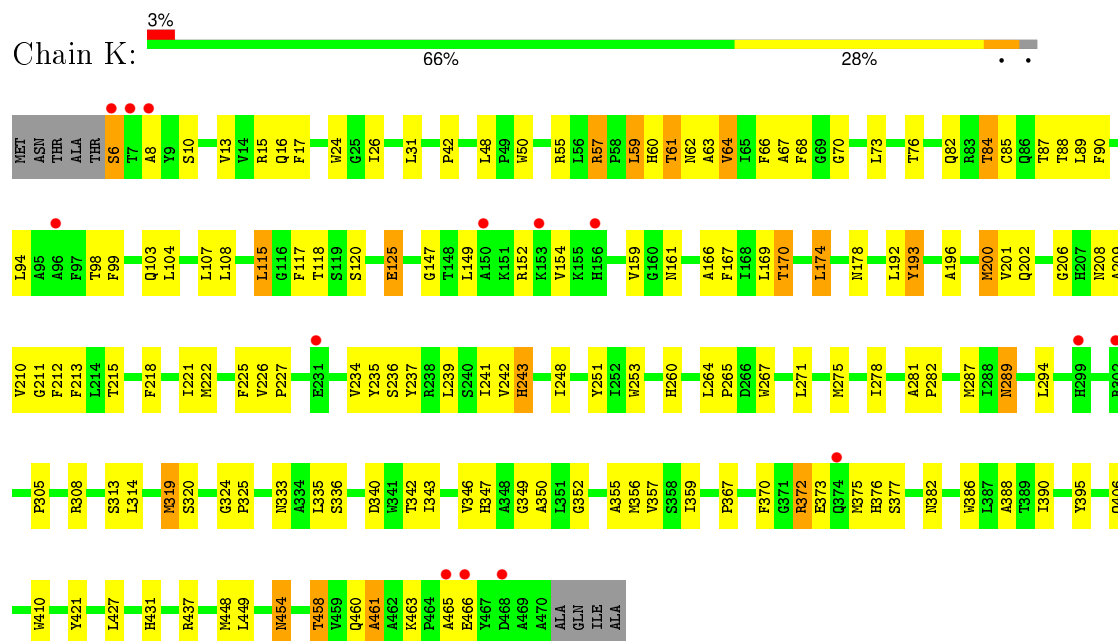
- Chain D:
-
- 64% 29% 4%



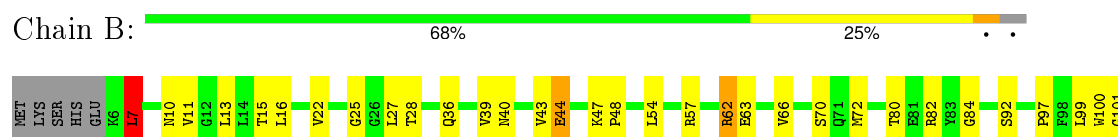
- Molecule 1: Cytochrome c oxidase, cbb3-type, subunit N



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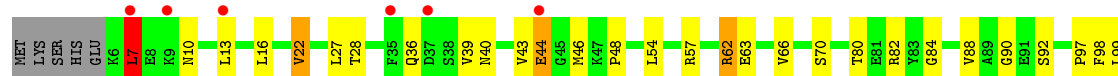


- Molecule 2: Cytochrome c oxidase, cbb3-type, subunit O





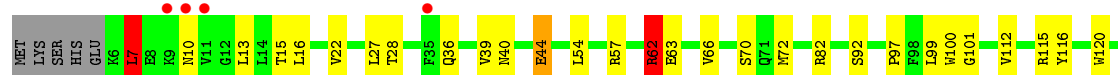
- Molecule 2: Cytochrome c oxidase, cbb3-type, subunit O



- Molecule 2: Cytochrome c oxidase, cbb3-type, subunit O



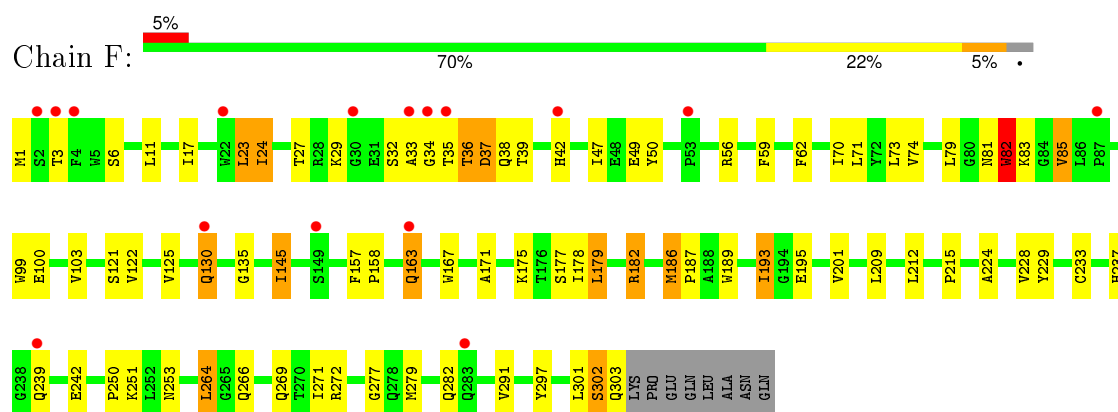
- Molecule 2: Cytochrome c oxidase, cbb3-type, subunit O



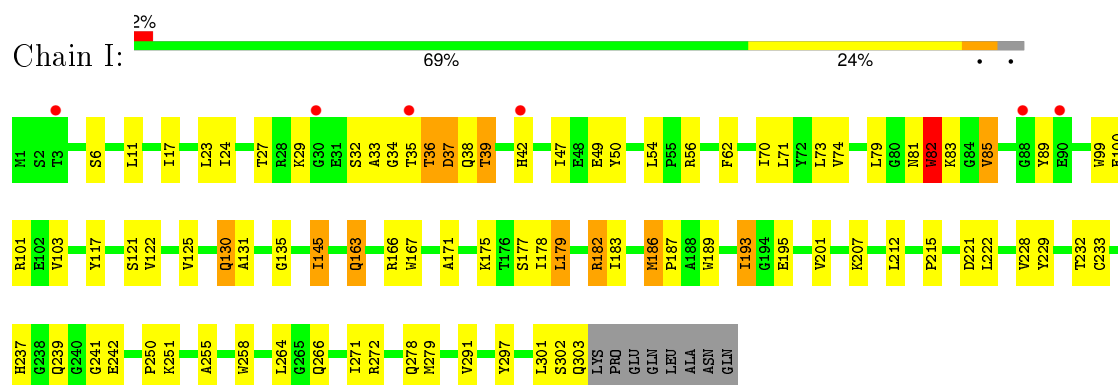
- Molecule 3: Cytochrome c oxidase, cbb3-type, subunit P



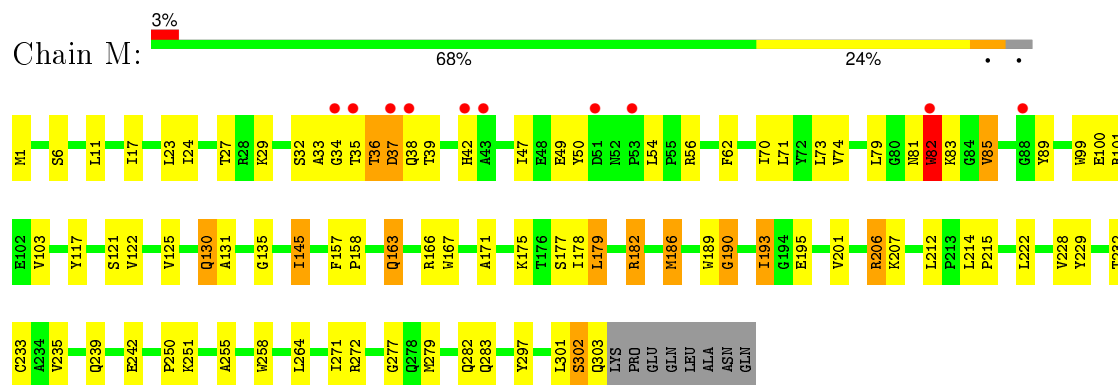
- Molecule 3: Cytochrome c oxidase, cbb3-type, subunit P



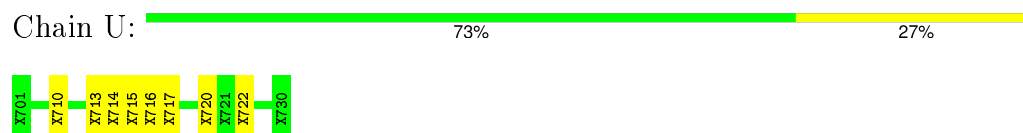
- Molecule 3: Cytochrome c oxidase, cbb3-type, subunit P



- Molecule 3: Cytochrome c oxidase, cbb3-type, subunit P

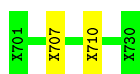


- Molecule 4: 30-mer peptide



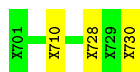
- Molecule 4: 30-mer peptide






- Molecule 4: 30-mer peptide

Chain Y:  90% 10%



- Molecule 4: 30-mer peptide

Chain Z:  80% 20%



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 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)	15.00 – 3.20 14.98 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.5 (15.00-3.20) 98.8 (14.98-3.00)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.6.0046	Depositor
R, R_{free}	0.189 , 0.223 0.198 , 0.232	Depositor DCC
R_{free} test set	5564 reflections (5.41%)	DCC
Wilson B-factor (Å ²)	87.0	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 82.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	2 of 131746 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	31690	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.58	0/3811	0.64	1/5210 (0.0%)
1	D	0.40	0/3791	0.54	0/5182
1	G	0.53	0/3804	0.60	0/5200
1	K	0.49	2/3804 (0.1%)	0.56	0/5200
2	B	0.68	0/1584	0.76	1/2146 (0.0%)
2	E	0.45	0/1584	0.64	1/2146 (0.0%)
2	H	0.62	0/1584	0.73	2/2146 (0.1%)
2	L	0.53	0/1584	0.69	2/2146 (0.1%)
3	C	0.61	0/2374	0.72	1/3225 (0.0%)
3	F	0.44	0/2374	0.59	0/3225
3	I	0.55	0/2374	0.66	0/3225
3	M	0.64	0/2374	0.71	1/3225 (0.0%)
All	All	0.54	2/31042 (0.0%)	0.64	9/42276 (0.0%)

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
2	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	6	SER	CB-OG	-9.55	1.29	1.42
1	K	6	SER	CA-CB	7.86	1.64	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	437	ARG	NE-CZ-NH2	-7.53	116.54	120.30
3	C	275	ARG	NE-CZ-NH1	-6.66	116.97	120.30
2	H	62	ARG	NE-CZ-NH1	5.60	123.10	120.30
2	L	62	ARG	NE-CZ-NH1	5.57	123.08	120.30
2	E	7	LEU	CA-CB-CG	5.39	127.69	115.30
3	M	206	ARG	NE-CZ-NH2	-5.37	117.61	120.30
2	B	7	LEU	CA-CB-CG	5.25	127.37	115.30
2	L	7	LEU	CA-CB-CG	5.09	127.01	115.30
2	H	7	LEU	CA-CB-CG	5.02	126.86	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	112	VAL	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3683	0	3663	121	0
1	D	3663	0	3644	117	0
1	G	3676	0	3656	120	0
1	K	3676	0	3656	111	0
2	B	1548	0	1526	45	0
2	E	1548	0	1526	45	0
2	H	1548	0	1526	48	0
2	L	1548	0	1526	36	0
3	C	2312	0	2237	68	1
3	F	2312	0	2237	69	0
3	I	2312	0	2237	67	1
3	M	2312	0	2237	65	0
4	U	150	0	33	6	0
4	X	150	0	33	2	0
4	Y	150	0	33	4	0
4	Z	150	0	35	4	0
5	A	86	0	60	11	0
5	D	86	0	60	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	G	86	0	60	13	0
5	K	86	0	60	12	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	1	0	0	0	0
7	B	1	0	0	0	0
7	D	1	0	0	0	0
7	E	1	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
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	0	0
9	D	5	0	0	0	0
9	G	5	0	0	0	0
9	K	5	0	0	0	0
10	B	43	0	30	3	0
10	C	86	0	60	10	0
10	E	43	0	30	2	0
10	F	86	0	60	17	0
10	H	43	0	30	4	0
10	I	86	0	60	6	0
10	L	43	0	30	2	0
10	M	86	0	60	9	0
11	C	13	0	0	4	0
11	F	13	0	0	10	0
11	I	13	0	0	6	0
11	M	13	0	0	3	0
All	All	31690	0	30405	858	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (858) 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:359:ILE:HD11	1:D:448:MET:HE1	1.18	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:359:ILE:HD11	1:K:448:MET:HE1	1.21	1.11
1:G:359:ILE:HD11	1:G:448:MET:HE1	1.19	1.11
1:A:359:ILE:HD11	1:A:448:MET:HE1	1.14	1.10
11:F:323:FC6:N24	3:I:215:PRO:HB3	1.66	1.10
1:G:166:ALA:O	1:G:170:THR:HG22	1.58	1.02
11:C:323:FC6:N24	3:M:215:PRO:HB3	1.73	1.02
3:F:193:ILE:HD11	3:F:228:VAL:HG11	1.40	1.01
3:C:186:MET:HG2	10:C:321:HEC:ND	1.76	1.00
1:D:359:ILE:HD11	1:D:448:MET:CE	1.91	0.99
2:B:193:GLN:HA	2:B:193:GLN:HE21	1.25	0.99
3:C:186:MET:HG2	10:C:321:HEC:C4D	1.92	0.99
1:A:166:ALA:O	1:A:170:THR:HG22	1.62	0.98
1:D:166:ALA:O	1:D:170:THR:HG22	1.63	0.98
2:H:193:GLN:HA	2:H:193:GLN:HE21	1.30	0.97
1:K:166:ALA:O	1:K:170:THR:HG22	1.65	0.97
1:A:281:ALA:HB3	1:A:282:PRO:HD3	1.46	0.97
3:M:186:MET:HG2	10:M:321:HEC:ND	1.78	0.96
1:A:359:ILE:HD11	1:A:448:MET:CE	1.94	0.96
1:A:76:THR:HG21	1:A:221:ILE:HG12	1.48	0.96
1:G:281:ALA:HB3	1:G:282:PRO:HD3	1.48	0.95
5:A:502:HEM:HHC	5:A:502:HEM:HBB2	1.47	0.95
1:G:359:ILE:HD11	1:G:448:MET:CE	1.96	0.95
3:F:186:MET:HG2	10:F:321:HEC:C4D	1.97	0.95
5:D:502:HEM:HHC	5:D:502:HEM:HBB2	1.48	0.94
3:F:186:MET:HG2	10:F:321:HEC:ND	1.82	0.94
1:D:76:THR:HG21	1:D:221:ILE:HG12	1.50	0.93
2:H:157:MET:HE3	2:H:171:ASP:HB3	1.52	0.92
3:M:186:MET:HG2	10:M:321:HEC:C4D	1.98	0.92
1:K:359:ILE:HD11	1:K:448:MET:CE	1.99	0.91
1:K:76:THR:HG21	1:K:221:ILE:HG12	1.54	0.90
1:G:24:TRP:HE1	1:G:103:GLN:HE22	1.20	0.90
3:I:193:ILE:HD11	3:I:228:VAL:HG11	1.51	0.89
1:D:24:TRP:HE1	1:D:103:GLN:HE22	1.16	0.89
1:A:335:LEU:HD22	4:U:710:UNK:CB	2.02	0.89
3:F:167:TRP:CE2	3:F:182:ARG:HG2	2.08	0.89
1:A:24:TRP:HE1	1:A:103:GLN:HE22	1.21	0.88
3:I:167:TRP:CE2	3:I:182:ARG:HG2	2.08	0.88
2:E:193:GLN:HA	2:E:193:GLN:HE21	1.35	0.88
2:L:193:GLN:HE21	2:L:193:GLN:HA	1.38	0.88
2:B:157:MET:HE1	2:B:171:ASP:HB3	1.55	0.88
3:M:193:ILE:HD11	3:M:228:VAL:HG11	1.52	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:167:TRP:CE2	3:C:182:ARG:HG2	2.10	0.87
3:M:167:TRP:CE2	3:M:182:ARG:HG2	2.10	0.86
5:G:502:HEM:HHC	5:G:502:HEM:HBB2	1.55	0.86
2:E:157:MET:HE3	2:E:171:ASP:HB3	1.58	0.85
2:L:157:MET:HE1	2:L:171:ASP:HB3	1.56	0.85
3:I:186:MET:HG2	10:I:321:HEC:C4D	1.94	0.85
1:K:24:TRP:HE1	1:K:103:GLN:HE22	1.22	0.84
3:C:193:ILE:HD11	3:C:228:VAL:HG11	1.60	0.84
1:K:281:ALA:HB3	1:K:282:PRO:HD3	1.60	0.84
1:D:281:ALA:HB3	1:D:282:PRO:HD3	1.60	0.83
3:C:215:PRO:HB3	11:M:323:FC6:N24	1.94	0.83
5:K:502:HEM:HHC	5:K:502:HEM:HBB2	1.61	0.82
1:G:76:THR:HG21	1:G:221:ILE:HG12	1.59	0.82
2:E:116:TYR:HE2	3:F:145:ILE:HG21	1.45	0.82
1:K:335:LEU:HD22	4:Z:710:UNK:CB	2.10	0.82
1:A:10:SER:H	1:A:82:GLN:HE22	1.28	0.81
1:G:10:SER:H	1:G:82:GLN:HE22	1.27	0.80
1:D:10:SER:H	1:D:82:GLN:HE22	1.29	0.80
1:G:170:THR:HG21	1:G:212:PHE:CD2	2.16	0.80
5:K:502:HEM:HBC2	5:K:502:HEM:HHD	1.65	0.78
1:G:335:LEU:HD22	4:Y:710:UNK:CB	2.14	0.78
1:D:85:CYS:HB2	1:D:152:ARG:HB2	1.65	0.77
1:K:85:CYS:HB2	1:K:152:ARG:HB2	1.66	0.77
3:I:207:LYS:HD3	3:I:222:LEU:HD21	1.67	0.77
1:A:63:ALA:O	1:A:67:ALA:HB3	1.84	0.77
1:G:85:CYS:HB2	1:G:152:ARG:HB2	1.67	0.77
1:G:325:PRO:HD3	5:G:501:HEM:HBB2	1.68	0.75
1:K:10:SER:H	1:K:82:GLN:HE22	1.35	0.75
1:A:170:THR:HG21	1:A:212:PHE:CD2	2.22	0.74
1:D:170:THR:HG21	1:D:212:PHE:CD2	2.23	0.74
5:G:502:HEM:HBC2	5:G:502:HEM:HHD	1.68	0.74
1:K:170:THR:HG21	1:K:212:PHE:CD2	2.22	0.74
3:F:215:PRO:HB3	11:I:323:FC6:N24	2.02	0.74
1:A:85:CYS:HB2	1:A:152:ARG:HB2	1.68	0.73
1:D:335:LEU:HD22	4:X:710:UNK:CB	2.18	0.73
5:A:502:HEM:HBC2	5:A:502:HEM:HHD	1.70	0.73
5:D:502:HEM:HBC2	5:D:502:HEM:HHD	1.71	0.73
1:A:325:PRO:HD3	5:A:501:HEM:HBB2	1.71	0.72
1:D:63:ALA:O	1:D:67:ALA:HB3	1.88	0.72
1:G:355:ALA:O	1:G:359:ILE:HG12	1.90	0.72
1:D:325:PRO:HD3	5:D:501:HEM:HBB2	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:63:ALA:O	1:G:67:ALA:HB3	1.90	0.71
2:B:128:PRO:HD2	2:B:129:ARG:HH21	1.55	0.71
3:M:17:ILE:HG21	3:M:70:ILE:HD11	1.72	0.71
2:E:116:TYR:CE2	3:F:145:ILE:HG21	2.24	0.71
2:L:57:ARG:NH2	2:L:97:PRO:O	2.23	0.71
1:D:356:MET:HE3	1:D:388:ALA:HB1	1.72	0.71
1:K:31:LEU:HD11	1:K:59:LEU:HD13	1.72	0.71
1:A:356:MET:HE3	1:A:388:ALA:HB1	1.73	0.70
1:A:61:THR:HG22	1:A:62:ASN:HD22	1.55	0.70
3:F:17:ILE:HG21	3:F:70:ILE:HD11	1.73	0.70
2:B:7:LEU:HA	2:B:10:ASN:HD22	1.57	0.70
3:F:271:ILE:HG12	10:F:321:HEC:HMB2	1.72	0.70
2:B:57:ARG:NH2	2:B:97:PRO:O	2.25	0.70
1:K:63:ALA:O	1:K:67:ALA:HB3	1.91	0.69
1:K:325:PRO:HD3	5:K:501:HEM:HBB2	1.73	0.69
2:E:62:ARG:HH22	2:E:184:GLU:CD	1.96	0.69
3:C:189:TRP:O	3:C:193:ILE:HG22	1.92	0.69
1:G:253:TRP:CH2	2:H:28:THR:HG21	2.27	0.69
1:D:31:LEU:HD11	1:D:59:LEU:HD13	1.75	0.68
3:F:229:TYR:HE1	3:F:239:GLN:HA	1.58	0.68
1:K:421:TYR:O	2:L:82:ARG:NH2	2.27	0.68
3:C:195:GLU:OE2	3:C:272:ARG:NH1	2.27	0.68
3:I:17:ILE:HG21	3:I:70:ILE:HD11	1.76	0.67
1:K:64:VAL:HG11	5:K:502:HEM:C4C	2.28	0.67
2:H:57:ARG:NH2	2:H:97:PRO:O	2.27	0.67
1:G:352:GLY:O	1:G:356:MET:HG3	1.93	0.67
1:A:340:ASP:H	1:A:406:GLN:HE22	1.42	0.67
1:A:349:GLY:HA3	5:A:501:HEM:HAC	1.76	0.67
2:E:44:GLU:HB3	2:E:202:LYS:HB2	1.77	0.67
1:D:355:ALA:O	1:D:359:ILE:HG12	1.94	0.66
3:M:195:GLU:OE2	3:M:272:ARG:NH1	2.29	0.66
1:G:64:VAL:HG11	5:G:502:HEM:C4C	2.31	0.66
2:H:116:TYR:HE2	3:I:145:ILE:HG21	1.61	0.66
1:G:61:THR:HG22	1:G:62:ASN:HD22	1.59	0.66
1:D:253:TRP:CH2	2:E:28:THR:HG21	2.31	0.66
3:I:279:MET:HB2	10:I:322:HEC:C4D	2.25	0.66
1:K:355:ALA:O	1:K:359:ILE:HG12	1.95	0.66
3:I:36:THR:O	3:I:37:ASP:HB2	1.93	0.66
1:D:359:ILE:CD1	1:D:448:MET:HE1	2.12	0.66
1:K:349:GLY:HA3	5:K:501:HEM:HAC	1.78	0.66
1:K:61:THR:HG22	1:K:62:ASN:HD22	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:229:TYR:HE1	3:M:239:GLN:HA	1.60	0.65
1:G:10:SER:N	1:G:82:GLN:HE22	1.94	0.65
3:M:36:THR:O	3:M:37:ASP:HB2	1.96	0.65
1:D:17:PHE:CZ	1:D:99:PHE:HA	2.31	0.65
2:H:7:LEU:HA	2:H:10:ASN:HD22	1.61	0.65
1:A:76:THR:HG21	1:A:221:ILE:CG1	2.23	0.65
1:G:347:HIS:HA	1:G:350:ALA:HB3	1.78	0.65
1:G:356:MET:CE	1:G:388:ALA:HB1	2.27	0.65
3:C:17:ILE:HG21	3:C:70:ILE:HD11	1.78	0.65
2:H:44:GLU:HB3	2:H:202:LYS:HB2	1.78	0.65
3:M:130:GLN:HE21	3:M:130:GLN:HA	1.61	0.65
1:D:352:GLY:O	1:D:356:MET:HG3	1.97	0.65
1:A:355:ALA:O	1:A:359:ILE:HG12	1.97	0.65
3:F:189:TRP:CZ2	10:F:321:HEC:HMC2	2.32	0.65
3:C:189:TRP:CZ2	10:C:321:HEC:HMC2	2.32	0.65
1:A:31:LEU:HD11	1:A:59:LEU:HD13	1.77	0.65
2:E:7:LEU:HA	2:E:10:ASN:HD22	1.61	0.65
3:F:36:THR:O	3:F:37:ASP:HB2	1.97	0.64
3:I:189:TRP:O	3:I:193:ILE:HG22	1.96	0.64
1:A:17:PHE:CZ	1:A:99:PHE:HA	2.33	0.64
1:A:253:TRP:CH2	2:B:28:THR:HG21	2.31	0.64
2:L:7:LEU:HA	2:L:10:ASN:HD22	1.60	0.64
1:D:356:MET:CE	1:D:388:ALA:HB1	2.26	0.64
1:K:253:TRP:CH2	2:L:28:THR:HG21	2.32	0.64
1:K:340:ASP:H	1:K:406:GLN:HE22	1.44	0.64
2:B:44:GLU:HB3	2:B:202:LYS:HB2	1.80	0.64
1:A:82:GLN:NE2	1:A:89:LEU:H	1.96	0.64
1:A:421:TYR:O	2:B:82:ARG:NH2	2.31	0.64
3:C:279:MET:HB2	10:C:322:HEC:C4D	2.27	0.64
2:L:44:GLU:HB3	2:L:202:LYS:HB2	1.79	0.64
1:K:352:GLY:O	1:K:356:MET:HG3	1.98	0.64
2:H:193:GLN:HA	2:H:193:GLN:NE2	2.09	0.64
1:K:356:MET:CE	1:K:388:ALA:HB1	2.29	0.63
1:K:386:TRP:O	1:K:390:ILE:HG12	1.99	0.63
2:B:62:ARG:NH1	2:B:63:GLU:OE2	2.28	0.63
3:I:183:ILE:HG12	3:I:278:GLN:HG2	1.80	0.63
1:D:76:THR:HG21	1:D:221:ILE:CG1	2.24	0.63
2:E:128:PRO:HD2	2:E:129:ARG:HH21	1.63	0.63
2:B:116:TYR:HE2	3:C:145:ILE:HG21	1.63	0.63
1:D:10:SER:N	1:D:82:GLN:HE22	1.95	0.63
2:E:57:ARG:NH2	2:E:97:PRO:O	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:229:TYR:HE1	3:C:239:GLN:HA	1.62	0.63
1:D:386:TRP:O	1:D:390:ILE:HG12	1.99	0.63
1:G:386:TRP:O	1:G:390:ILE:HG12	1.98	0.63
3:F:195:GLU:OE2	3:F:272:ARG:NH1	2.30	0.63
2:L:62:ARG:HH22	2:L:184:GLU:CD	2.01	0.63
3:C:36:THR:O	3:C:37:ASP:HB2	1.98	0.63
3:F:193:ILE:HD11	3:F:228:VAL:CG1	2.24	0.63
2:B:193:GLN:HA	2:B:193:GLN:NE2	2.06	0.63
1:G:356:MET:HE3	1:G:388:ALA:HB1	1.79	0.63
1:K:10:SER:N	1:K:82:GLN:HE22	1.97	0.63
1:D:64:VAL:HG11	5:D:502:HEM:C4C	2.34	0.62
1:G:17:PHE:CZ	1:G:99:PHE:HA	2.34	0.62
1:D:82:GLN:NE2	1:D:89:LEU:H	1.97	0.62
2:L:62:ARG:NH1	2:L:63:GLU:OE2	2.32	0.62
3:I:130:GLN:HE21	3:I:130:GLN:HA	1.62	0.62
2:L:116:TYR:HE2	3:M:145:ILE:HG21	1.63	0.62
1:A:10:SER:N	1:A:82:GLN:HE22	1.97	0.62
3:I:266:GLN:NE2	11:I:323:FC6:N11	2.47	0.62
3:M:279:MET:HB2	10:M:322:HEC:C4D	2.29	0.62
3:F:189:TRP:O	3:F:193:ILE:HG22	1.99	0.62
3:F:279:MET:HB2	10:F:322:HEC:C4D	2.30	0.62
3:C:130:GLN:HE21	3:C:130:GLN:HA	1.63	0.62
1:A:346:VAL:HG22	5:A:501:HEM:C2D	2.34	0.62
1:D:421:TYR:O	2:E:82:ARG:NH2	2.33	0.62
1:K:82:GLN:NE2	1:K:89:LEU:H	1.98	0.62
1:A:178:ASN:HD22	1:A:201:VAL:HG12	1.65	0.62
1:K:76:THR:HG21	1:K:221:ILE:CG1	2.29	0.61
3:I:271:ILE:HG12	10:I:321:HEC:HMB2	1.82	0.61
1:G:349:GLY:HA3	5:G:501:HEM:HAC	1.81	0.61
1:K:356:MET:HE3	1:K:388:ALA:HB1	1.81	0.61
1:A:372:ARG:NH1	1:A:461:ALA:HB1	2.14	0.61
1:A:356:MET:CE	1:A:388:ALA:HB1	2.29	0.61
2:H:128:PRO:HD2	2:H:129:ARG:HH21	1.65	0.61
2:B:138:PRO:HD3	10:B:211:HEC:HBC3	1.81	0.61
2:H:138:PRO:HD3	10:H:211:HEC:HBC3	1.82	0.61
3:C:277:GLY:HA3	10:C:322:HEC:O1D	2.01	0.61
1:D:347:HIS:HA	1:D:350:ALA:HB3	1.82	0.61
1:G:234:VAL:HB	3:I:49:GLU:HB3	1.82	0.61
1:A:352:GLY:O	1:A:356:MET:HG3	2.00	0.61
3:M:74:VAL:O	3:M:82:TRP:CZ3	2.53	0.61
1:D:82:GLN:HE21	1:D:89:LEU:H	1.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:349:GLY:HA3	5:D:501:HEM:HAC	1.82	0.61
2:B:62:ARG:HH22	2:B:184:GLU:CD	2.04	0.61
1:K:17:PHE:CZ	1:K:99:PHE:HA	2.36	0.61
1:A:64:VAL:HG11	5:A:502:HEM:C4C	2.36	0.61
1:K:340:ASP:H	1:K:406:GLN:NE2	1.99	0.61
3:F:130:GLN:HA	3:F:130:GLN:HE21	1.65	0.61
1:K:239:LEU:O	1:K:243:HIS:HB3	2.01	0.60
3:I:229:TYR:HE1	3:I:239:GLN:HA	1.66	0.60
1:D:10:SER:H	1:D:82:GLN:NE2	1.99	0.60
1:A:431:HIS:HD2	2:B:136:LYS:NZ	1.99	0.60
1:D:372:ARG:NH1	1:D:461:ALA:HB1	2.16	0.60
2:H:62:ARG:HH22	2:H:184:GLU:CD	2.05	0.60
1:G:239:LEU:HD23	1:G:289:ASN:HD22	1.66	0.60
1:K:222:MET:HG3	1:K:314:LEU:HD21	1.83	0.60
1:G:31:LEU:HD11	1:G:59:LEU:HD13	1.81	0.60
1:A:222:MET:HG3	1:A:314:LEU:HD21	1.83	0.60
1:A:281:ALA:HB3	1:A:282:PRO:CD	2.26	0.60
1:A:359:ILE:CD1	1:A:448:MET:HE1	2.10	0.60
2:E:116:TYR:HE2	3:F:145:ILE:CG2	2.11	0.60
3:F:189:TRP:HZ2	10:F:321:HEC:HMC2	1.66	0.60
1:K:343:ILE:HG12	5:K:502:HEM:HBA2	1.84	0.60
1:G:372:ARG:NH1	1:G:461:ALA:HB1	2.16	0.60
3:C:189:TRP:HZ2	10:C:321:HEC:HMC2	1.67	0.60
2:B:193:GLN:HE21	2:B:193:GLN:CA	2.08	0.60
1:K:82:GLN:HE21	1:K:89:LEU:H	1.49	0.60
3:I:195:GLU:OE2	3:I:272:ARG:NH1	2.35	0.60
3:C:32:SER:O	3:C:34:GLY:N	2.35	0.60
11:F:323:FC6:C24	3:I:215:PRO:HB3	2.27	0.59
2:H:62:ARG:NH1	2:H:63:GLU:OE2	2.33	0.59
3:M:73:LEU:HD22	3:M:79:LEU:HG	1.84	0.59
1:A:82:GLN:HE21	1:A:89:LEU:H	1.50	0.59
1:A:340:ASP:H	1:A:406:GLN:NE2	1.99	0.59
2:E:80:THR:HG21	3:F:99:TRP:HZ2	1.67	0.59
1:A:239:LEU:HD23	1:A:289:ASN:HD22	1.66	0.59
1:A:239:LEU:O	1:A:243:HIS:HB3	2.03	0.59
1:G:375:MET:HE2	1:G:375:MET:HA	1.85	0.59
3:F:73:LEU:HD22	3:F:79:LEU:HG	1.85	0.59
1:K:454:ASN:O	1:K:458:THR:HG23	2.03	0.59
1:G:82:GLN:NE2	1:G:89:LEU:H	2.00	0.59
1:G:76:THR:HG21	1:G:221:ILE:CG1	2.32	0.59
1:D:335:LEU:HD13	4:X:707:UNK:HA	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:128:PRO:HD2	2:L:129:ARG:HH21	1.68	0.58
1:G:178:ASN:HD22	1:G:201:VAL:HG12	1.69	0.58
3:I:189:TRP:CZ2	10:I:321:HEC:HMC2	2.38	0.58
3:I:73:LEU:HD22	3:I:79:LEU:HG	1.85	0.58
2:L:62:ARG:HG3	2:L:63:GLU:N	2.19	0.58
3:F:74:VAL:O	3:F:82:TRP:CZ3	2.57	0.58
3:C:215:PRO:HG3	11:M:323:FC6:C21	2.34	0.58
3:C:74:VAL:O	3:C:82:TRP:CZ3	2.57	0.57
3:M:207:LYS:HD3	3:M:222:LEU:HD21	1.85	0.57
1:D:340:ASP:H	1:D:406:GLN:NE2	2.02	0.57
1:K:347:HIS:HA	1:K:350:ALA:HB3	1.85	0.57
1:A:386:TRP:O	1:A:390:ILE:HG12	2.03	0.57
1:G:346:VAL:HG22	5:G:501:HEM:C2D	2.39	0.57
1:A:233:PRO:HG2	3:C:50:TYR:CZ	2.39	0.57
2:E:138:PRO:HD3	10:E:211:HEC:HBC3	1.85	0.57
3:C:271:ILE:HG12	10:C:321:HEC:HMB2	1.87	0.57
3:I:266:GLN:HG2	11:I:323:FC6:C22	2.34	0.57
1:K:174:LEU:HD21	1:K:208:ASN:HB3	1.86	0.57
1:A:281:ALA:CB	1:A:282:PRO:HD3	2.29	0.57
1:K:227:PRO:HB2	3:M:47:ILE:HD12	1.87	0.57
1:D:431:HIS:HD2	2:E:136:LYS:NZ	2.03	0.57
1:D:375:MET:HA	1:D:375:MET:HE2	1.87	0.57
1:D:340:ASP:H	1:D:406:GLN:HE22	1.52	0.57
3:I:74:VAL:O	3:I:82:TRP:CZ3	2.58	0.57
1:G:239:LEU:O	1:G:243:HIS:HB3	2.05	0.56
1:G:342:THR:O	1:G:346:VAL:HG23	2.05	0.56
3:C:178:ILE:HG12	10:C:322:HEC:HMB2	1.87	0.56
1:D:61:THR:HG22	1:D:62:ASN:HD22	1.69	0.56
1:A:418:THR:OG1	3:C:137:ARG:HD2	2.05	0.56
1:A:375:MET:HA	1:A:375:MET:HE2	1.87	0.56
2:L:138:PRO:HD3	10:L:211:HEC:HBC3	1.87	0.56
2:B:177:ASP:OD1	2:B:177:ASP:N	2.38	0.56
1:G:82:GLN:HE21	1:G:88:THR:HA	1.71	0.56
1:K:375:MET:HE2	1:K:375:MET:HA	1.87	0.56
1:K:13:VAL:HA	1:K:16:GLN:HE21	1.70	0.56
1:A:13:VAL:HA	1:A:16:GLN:HE21	1.69	0.56
1:D:239:LEU:HD23	1:D:289:ASN:HD22	1.70	0.56
3:M:239:GLN:N	3:M:239:GLN:OE1	2.36	0.56
1:D:346:VAL:HG22	5:D:501:HEM:C2D	2.39	0.56
3:F:187:PRO:HG2	3:F:189:TRP:CZ2	2.40	0.56
3:C:6:SER:OG	3:C:81:ASN:HB2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:189:TRP:CZ2	10:M:321:HEC:HMC2	2.41	0.55
2:E:193:GLN:HA	2:E:193:GLN:NE2	2.13	0.55
2:E:117:SER:H	10:F:322:HEC:HBC1	1.72	0.55
1:G:10:SER:H	1:G:82:GLN:NE2	1.98	0.55
3:I:38:GLN:O	3:I:50:TYR:HD2	1.88	0.55
1:G:343:ILE:HG12	5:G:502:HEM:HBA2	1.88	0.55
1:D:62:ASN:HD21	1:D:125:GLU:HG3	1.72	0.55
1:A:234:VAL:HB	3:C:49:GLU:HB3	1.87	0.55
3:M:277:GLY:HA3	10:M:322:HEC:O1D	2.06	0.55
1:G:237:TYR:CE2	1:G:241:ILE:HD11	2.41	0.55
1:G:115:LEU:HB3	1:G:117:PHE:CE2	2.42	0.55
1:D:76:THR:HG23	1:D:225:PHE:HE1	1.72	0.55
1:D:239:LEU:O	1:D:243:HIS:HB3	2.06	0.55
3:M:38:GLN:O	3:M:50:TYR:HD2	1.89	0.55
1:D:367:PRO:HD3	1:D:375:MET:HE3	1.89	0.55
1:D:227:PRO:HB2	3:F:47:ILE:HD12	1.88	0.55
3:M:178:ILE:HG12	10:M:322:HEC:HMB2	1.89	0.55
1:A:335:LEU:CD2	4:U:710:UNK:CB	2.82	0.55
1:K:239:LEU:HD23	1:K:289:ASN:HD22	1.72	0.55
1:A:82:GLN:HE21	1:A:88:THR:HA	1.72	0.55
1:D:174:LEU:HD21	1:D:208:ASN:HB3	1.88	0.55
1:G:222:MET:HG3	1:G:314:LEU:HD21	1.89	0.55
1:G:281:ALA:HB3	1:G:282:PRO:CD	2.28	0.55
1:G:82:GLN:HE21	1:G:89:LEU:H	1.55	0.55
1:A:10:SER:H	1:A:82:GLN:NE2	2.01	0.54
2:B:62:ARG:HG3	2:B:63:GLU:N	2.23	0.54
1:D:234:VAL:HB	3:F:49:GLU:HB3	1.88	0.54
11:F:323:FC6:C21	3:I:215:PRO:HG3	2.38	0.54
3:C:186:MET:HG2	10:C:321:HEC:CHA	2.36	0.54
1:G:10:SER:HB2	1:G:88:THR:HG23	1.88	0.54
1:D:222:MET:HG3	1:D:314:LEU:HD21	1.88	0.54
3:F:6:SER:OG	3:F:81:ASN:HB2	2.06	0.54
1:K:234:VAL:HB	3:M:49:GLU:HB3	1.90	0.54
1:D:13:VAL:HA	1:D:16:GLN:HE21	1.72	0.54
1:G:211:GLY:O	1:G:215:THR:HB	2.08	0.54
1:K:10:SER:H	1:K:82:GLN:NE2	2.03	0.54
1:K:149:LEU:HD21	1:K:161:ASN:HD22	1.73	0.54
1:K:431:HIS:HD2	2:L:136:LYS:NZ	2.04	0.54
3:F:178:ILE:HG12	10:F:322:HEC:HMB2	1.89	0.54
2:H:116:TYR:CE2	3:I:145:ILE:HG21	2.41	0.54
3:I:6:SER:OG	3:I:81:ASN:HB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:32:SER:O	3:F:34:GLY:N	2.41	0.54
1:K:237:TYR:CE2	1:K:241:ILE:HD11	2.42	0.54
3:C:135:GLY:HA3	3:C:297:TYR:HB2	1.90	0.54
3:F:266:GLN:NE2	11:F:323:FC6:N11	2.56	0.53
11:C:323:FC6:C24	3:M:215:PRO:HB3	2.35	0.53
1:K:6:SER:C	1:K:8:ALA:H	2.11	0.53
1:D:84:THR:CG2	1:D:161:ASN:HD21	2.21	0.53
3:I:32:SER:O	3:I:34:GLY:N	2.40	0.53
3:F:266:GLN:HG3	11:F:323:FC6:N22	2.24	0.53
3:M:271:ILE:HG12	10:M:321:HEC:HMB2	1.89	0.53
5:D:502:HEM:HBB2	5:D:502:HEM:CHC	2.29	0.53
1:A:55:ARG:NH2	2:B:62:ARG:HD2	2.23	0.53
1:G:421:TYR:O	2:H:82:ARG:NH2	2.41	0.53
3:M:32:SER:O	3:M:34:GLY:N	2.41	0.53
3:F:135:GLY:HA3	3:F:297:TYR:HB2	1.89	0.53
1:D:454:ASN:O	1:D:458:THR:HG23	2.08	0.53
3:I:167:TRP:CD2	3:I:182:ARG:HG2	2.42	0.53
1:A:61:THR:HG22	1:A:62:ASN:ND2	2.23	0.53
1:K:178:ASN:HD22	1:K:201:VAL:HG12	1.73	0.53
2:L:177:ASP:N	2:L:177:ASP:OD1	2.42	0.53
2:B:57:ARG:NH1	2:B:99:LEU:HD12	2.23	0.53
1:K:346:VAL:HG22	5:K:501:HEM:C2D	2.43	0.53
3:C:239:GLN:OE1	3:C:239:GLN:N	2.40	0.53
1:K:372:ARG:NH1	1:K:461:ALA:HB1	2.23	0.53
1:D:82:GLN:HE21	1:D:88:THR:HA	1.74	0.53
1:G:454:ASN:O	1:G:458:THR:HG23	2.08	0.53
2:E:70:SER:HA	2:E:101:GLY:HA3	1.91	0.53
1:K:10:SER:HB2	1:K:88:THR:HG23	1.91	0.52
1:A:395:TYR:CZ	1:A:437:ARG:HD2	2.45	0.52
3:C:227:ASN:OD1	2:H:201:ASN:HB2	2.09	0.52
3:F:186:MET:HG2	10:F:321:HEC:CHA	2.38	0.52
3:F:167:TRP:CD2	3:F:182:ARG:HG2	2.45	0.52
3:I:122:VAL:HB	3:I:171:ALA:HB1	1.91	0.52
3:F:38:GLN:O	3:F:50:TYR:HD2	1.92	0.52
3:M:189:TRP:HZ2	10:M:321:HEC:HMC2	1.75	0.52
1:G:13:VAL:HA	1:G:16:GLN:HE21	1.73	0.52
3:C:242:GLU:CD	3:C:242:GLU:H	2.11	0.52
3:C:189:TRP:CZ3	3:C:232:THR:HG21	2.45	0.52
2:E:161:ARG:HA	2:E:165:VAL:O	2.10	0.52
1:A:66:PHE:O	1:A:70:GLY:HA3	2.09	0.52
1:G:281:ALA:CB	1:G:282:PRO:HD3	2.31	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:239:GLN:N	3:I:239:GLN:OE1	2.39	0.52
1:A:90:PHE:CD1	1:A:147:GLY:HA3	2.45	0.52
1:G:395:TYR:CZ	1:G:437:ARG:HD2	2.45	0.52
1:A:211:GLY:O	1:A:215:THR:HB	2.09	0.52
2:H:161:ARG:HA	2:H:165:VAL:O	2.09	0.52
2:E:62:ARG:HG3	2:E:63:GLU:N	2.24	0.52
2:H:62:ARG:HG3	2:H:63:GLU:N	2.24	0.52
1:G:367:PRO:HD3	1:G:375:MET:HE3	1.91	0.52
2:L:193:GLN:NE2	2:L:193:GLN:HA	2.17	0.52
2:H:116:TYR:HE2	3:I:145:ILE:CG2	2.22	0.52
1:A:84:THR:CG2	1:A:161:ASN:HD21	2.23	0.52
1:G:202:GLN:O	1:G:206:GLY:N	2.35	0.52
2:E:63:GLU:HA	2:E:63:GLU:OE1	2.10	0.52
1:D:61:THR:HG22	1:D:62:ASN:N	2.25	0.51
3:I:242:GLU:H	3:I:242:GLU:CD	2.12	0.51
2:E:62:ARG:NH1	2:E:63:GLU:OE2	2.38	0.51
3:I:178:ILE:HG12	10:I:322:HEC:HMB2	1.92	0.51
3:C:73:LEU:HD22	3:C:79:LEU:HG	1.92	0.51
1:G:227:PRO:HB2	3:I:47:ILE:HD12	1.92	0.51
3:I:187:PRO:HG2	3:I:189:TRP:CZ2	2.44	0.51
1:G:26:ILE:HD12	1:G:449:LEU:HD23	1.92	0.51
1:G:174:LEU:HD21	1:G:208:ASN:HB3	1.92	0.51
2:E:177:ASP:N	2:E:177:ASP:OD1	2.44	0.51
3:I:177:SER:HA	3:I:182:ARG:HD2	1.92	0.51
2:H:63:GLU:OE1	2:H:63:GLU:HA	2.10	0.51
3:M:193:ILE:HD11	3:M:228:VAL:CG1	2.33	0.51
3:M:122:VAL:HB	3:M:171:ALA:HB1	1.92	0.51
1:K:367:PRO:HD3	1:K:375:MET:HE3	1.92	0.51
1:D:149:LEU:HD21	1:D:161:ASN:HD22	1.76	0.51
2:B:36:GLN:O	2:B:40:ASN:ND2	2.43	0.51
1:G:149:LEU:HD21	1:G:161:ASN:HD22	1.75	0.51
3:C:215:PRO:HG3	11:M:323:FC6:N25	2.25	0.51
1:G:377:SER:H	1:G:454:ASN:HD21	1.58	0.51
3:M:99:TRP:O	3:M:103:VAL:HG23	2.10	0.51
1:A:10:SER:HB2	1:A:88:THR:HG23	1.92	0.51
2:L:116:TYR:CE2	3:M:145:ILE:HG21	2.45	0.51
1:D:410:TRP:O	2:E:82:ARG:NH1	2.42	0.51
2:L:129:ARG:HD3	2:L:135:SER:O	2.11	0.51
1:D:211:GLY:O	1:D:215:THR:HB	2.10	0.51
2:L:116:TYR:HE2	3:M:145:ILE:CG2	2.24	0.51
3:I:302:SER:O	3:I:303:GLN:HB3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:10:SER:HB2	1:D:88:THR:HG23	1.91	0.50
1:D:178:ASN:HD22	1:D:201:VAL:HG12	1.75	0.50
2:L:72:MET:HE3	2:L:100:TRP:CD2	2.46	0.50
1:A:61:THR:HG22	1:A:62:ASN:N	2.26	0.50
1:A:410:TRP:O	2:B:82:ARG:NH1	2.42	0.50
1:A:15:ARG:HG2	1:A:370:PHE:CZ	2.47	0.50
3:C:163:GLN:HE21	3:C:163:GLN:HA	1.77	0.50
1:A:174:LEU:HD21	1:A:208:ASN:HB3	1.93	0.50
1:A:377:SER:H	1:A:454:ASN:HD21	1.60	0.50
1:A:454:ASN:O	1:A:458:THR:HG23	2.11	0.50
2:L:161:ARG:HA	2:L:165:VAL:O	2.11	0.50
2:B:70:SER:HA	2:B:101:GLY:HA3	1.93	0.50
1:K:42:PRO:HG3	2:L:136:LYS:HD2	1.93	0.50
3:M:6:SER:OG	3:M:81:ASN:HB2	2.11	0.50
3:C:183:ILE:HG12	3:C:278:GLN:HG2	1.92	0.50
3:M:135:GLY:HA3	3:M:297:TYR:HB2	1.93	0.50
1:D:343:ILE:HG12	5:D:502:HEM:HBA2	1.92	0.50
2:H:88:VAL:HG12	2:H:90:GLY:H	1.76	0.50
1:G:242:VAL:HG22	3:I:27:THR:OG1	2.12	0.50
1:K:267:TRP:HE1	2:L:36:GLN:HE22	1.60	0.50
3:F:302:SER:O	3:F:303:GLN:HB3	2.11	0.50
1:A:310:LEU:O	1:A:313:SER:HB3	2.11	0.50
3:I:189:TRP:HZ2	10:I:321:HEC:HMC2	1.74	0.49
2:E:36:GLN:O	2:E:40:ASN:ND2	2.45	0.49
3:C:166:ARG:NH2	3:C:250:PRO:HG3	2.27	0.49
2:E:193:GLN:HE21	2:E:193:GLN:CA	2.18	0.49
1:K:218:PHE:CD2	1:K:221:ILE:HD12	2.47	0.49
3:I:135:GLY:HA3	3:I:297:TYR:HB2	1.93	0.49
3:F:266:GLN:HG3	11:F:323:FC6:C22	2.42	0.49
2:E:137:MET:HB2	10:E:211:HEC:C1D	2.42	0.49
1:K:395:TYR:CZ	1:K:437:ARG:HD2	2.48	0.49
2:L:70:SER:HA	2:L:101:GLY:HA3	1.93	0.49
3:C:122:VAL:HB	3:C:171:ALA:HB1	1.94	0.49
3:F:122:VAL:HB	3:F:171:ALA:HB1	1.95	0.49
1:K:82:GLN:HE21	1:K:88:THR:HA	1.77	0.49
1:D:237:TYR:CE2	1:D:241:ILE:HD11	2.47	0.49
11:F:323:FC6:N24	3:I:215:PRO:CB	2.58	0.49
1:K:372:ARG:HH11	1:K:372:ARG:HB2	1.78	0.49
1:A:196:ALA:HB3	2:B:39:VAL:HB	1.95	0.49
1:A:57:ARG:NH1	5:A:502:HEM:O2A	2.45	0.49
2:E:129:ARG:HD3	2:E:135:SER:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:TYR:O	1:A:289:ASN:ND2	2.46	0.49
2:L:36:GLN:O	2:L:40:ASN:ND2	2.46	0.48
1:A:347:HIS:HA	1:A:350:ALA:HB3	1.95	0.48
1:A:200:MET:HG3	1:A:264:LEU:HD11	1.95	0.48
1:A:13:VAL:HA	1:A:16:GLN:NE2	2.29	0.48
1:G:84:THR:CG2	1:G:161:ASN:HD21	2.25	0.48
1:G:94:LEU:O	1:G:98:THR:HG23	2.13	0.48
1:K:281:ALA:HB3	1:K:282:PRO:CD	2.39	0.48
2:H:57:ARG:NH1	2:H:99:LEU:HD12	2.28	0.48
2:B:80:THR:HA	2:B:84:GLY:O	2.13	0.48
3:C:167:TRP:CD2	3:C:182:ARG:HG2	2.48	0.48
3:M:229:TYR:CD2	3:M:233:CYS:HB2	2.48	0.48
1:G:15:ARG:HG2	1:G:370:PHE:CZ	2.48	0.48
4:U:715:UNK:O	4:U:716:UNK:C	2.61	0.48
1:A:115:LEU:HB3	1:A:117:PHE:CE2	2.49	0.48
1:A:76:THR:HG23	1:A:225:PHE:HE1	1.78	0.48
2:B:128:PRO:HD2	2:B:129:ARG:NH2	2.27	0.48
3:M:166:ARG:NH2	3:M:250:PRO:HG3	2.29	0.48
1:G:233:PRO:HG2	3:I:50:TYR:CZ	2.48	0.48
1:D:372:ARG:HH11	1:D:372:ARG:HB2	1.78	0.48
1:G:410:TRP:O	2:H:82:ARG:NH1	2.45	0.48
1:D:90:PHE:CD1	1:D:147:GLY:HA3	2.48	0.48
1:D:395:TYR:CZ	1:D:437:ARG:HD2	2.49	0.48
3:M:177:SER:HA	3:M:182:ARG:HD2	1.95	0.48
1:G:76:THR:HG23	1:G:225:PHE:HE1	1.78	0.48
2:H:177:ASP:N	2:H:177:ASP:OD1	2.47	0.48
1:A:343:ILE:HG12	5:A:502:HEM:HBA2	1.96	0.48
2:H:193:GLN:CA	2:H:193:GLN:HE21	2.14	0.47
2:E:116:TYR:HA	10:F:322:HEC:HBC3	1.96	0.47
1:K:84:THR:CG2	1:K:161:ASN:HD21	2.26	0.47
1:G:431:HIS:HD2	2:H:136:LYS:NZ	2.12	0.47
1:K:76:THR:HG23	1:K:225:PHE:HE1	1.77	0.47
1:G:61:THR:HG22	1:G:62:ASN:ND2	2.28	0.47
3:M:242:GLU:CD	3:M:242:GLU:H	2.18	0.47
3:I:163:GLN:HE21	3:I:163:GLN:HA	1.79	0.47
1:G:340:ASP:H	1:G:406:GLN:NE2	2.12	0.47
1:D:55:ARG:NH2	2:E:62:ARG:HD2	2.29	0.47
1:D:242:VAL:HG22	3:F:27:THR:OG1	2.14	0.47
1:D:66:PHE:O	1:D:70:GLY:HA3	2.15	0.47
1:A:169:LEU:HD11	2:B:15:THR:HG23	1.96	0.47
1:A:26:ILE:HD12	1:A:449:LEU:HD23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:90:PHE:CD1	1:K:147:GLY:HA3	2.49	0.47
3:I:266:GLN:HG3	11:I:323:FC6:N22	2.29	0.47
1:K:342:THR:O	1:K:346:VAL:HG23	2.14	0.47
1:A:242:VAL:HG22	3:C:27:THR:OG1	2.14	0.47
1:K:209:ALA:O	1:K:213:PHE:CB	2.63	0.47
1:K:26:ILE:HD12	1:K:449:LEU:HD23	1.96	0.47
3:C:99:TRP:O	3:C:103:VAL:HG23	2.15	0.47
3:I:229:TYR:CD2	3:I:233:CYS:HB2	2.50	0.47
1:K:196:ALA:HB3	2:L:39:VAL:HB	1.96	0.47
1:K:169:LEU:HD11	2:L:15:THR:HG23	1.95	0.47
2:H:70:SER:HA	2:H:101:GLY:HA3	1.96	0.47
3:C:215:PRO:CD	3:C:264:LEU:HD12	2.44	0.47
1:G:62:ASN:HD21	1:G:125:GLU:HG3	1.80	0.47
1:K:125:GLU:HG2	1:K:125:GLU:H	1.42	0.47
1:A:237:TYR:CE2	1:A:241:ILE:HD11	2.49	0.47
1:K:211:GLY:O	1:K:215:THR:HB	2.14	0.47
3:M:232:THR:O	3:M:235:VAL:HG23	2.14	0.47
3:I:193:ILE:HD11	3:I:228:VAL:CG1	2.36	0.47
3:C:38:GLN:O	3:C:50:TYR:HD2	1.97	0.47
2:B:72:MET:HE2	2:B:100:TRP:CD2	2.50	0.47
3:C:89:TYR:CD1	3:C:101:ARG:NH1	2.83	0.47
1:G:128:TRP:CG	1:G:129:PRO:HD3	2.50	0.47
1:K:193:TYR:CE1	1:K:201:VAL:HG11	2.49	0.47
1:G:226:VAL:HB	1:G:227:PRO:HD3	1.96	0.47
1:K:319:MET:HG3	1:K:320:SER:N	2.30	0.47
3:M:206:ARG:HD3	3:M:214:LEU:HD23	1.96	0.47
1:A:367:PRO:HG3	1:A:375:MET:HE2	1.96	0.47
1:G:169:LEU:HD11	2:H:15:THR:HG23	1.97	0.47
3:I:179:LEU:HD23	3:I:291:VAL:HG11	1.96	0.47
3:M:189:TRP:O	3:M:190:GLY:C	2.52	0.46
1:A:60:HIS:O	1:A:64:VAL:HB	2.15	0.46
3:M:177:SER:OG	3:M:182:ARG:NH1	2.44	0.46
1:K:235:TYR:O	1:K:289:ASN:ND2	2.47	0.46
1:A:346:VAL:HG22	5:A:501:HEM:C3D	2.50	0.46
1:K:376:HIS:CB	1:K:458:THR:HG22	2.45	0.46
1:K:242:VAL:HG22	3:M:27:THR:OG1	2.16	0.46
4:Y:728:UNK:C	4:Y:730:UNK:H	2.28	0.46
2:B:161:ARG:HA	2:B:165:VAL:O	2.15	0.46
3:F:177:SER:HA	3:F:182:ARG:HD2	1.98	0.46
1:D:346:VAL:HG22	5:D:501:HEM:C3D	2.49	0.46
2:E:57:ARG:NH1	2:E:99:LEU:HD12	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:64:VAL:HG11	5:K:502:HEM:CHD	2.45	0.46
2:B:128:PRO:HD3	2:B:139:SER:HA	1.97	0.46
3:C:177:SER:HA	3:C:182:ARG:HD2	1.97	0.46
1:G:376:HIS:CB	1:G:458:THR:HG22	2.46	0.46
1:D:26:ILE:HD12	1:D:449:LEU:HD23	1.97	0.46
3:I:99:TRP:O	3:I:103:VAL:HG23	2.15	0.46
1:K:115:LEU:HB3	1:K:117:PHE:CE2	2.50	0.46
2:B:48:PRO:HG3	2:B:166:PRO:HD2	1.96	0.46
1:A:202:GLN:O	1:A:206:GLY:N	2.44	0.46
3:F:242:GLU:H	3:F:242:GLU:CD	2.19	0.46
1:A:226:VAL:HB	1:A:227:PRO:HD3	1.96	0.46
1:D:15:ARG:HG2	1:D:370:PHE:CZ	2.51	0.46
1:G:218:PHE:HA	1:G:221:ILE:HG13	1.97	0.46
1:A:342:THR:O	1:A:346:VAL:HG23	2.16	0.46
1:K:377:SER:H	1:K:454:ASN:HD21	1.63	0.46
1:D:281:ALA:HB3	1:D:282:PRO:CD	2.39	0.46
1:A:149:LEU:HD21	1:A:161:ASN:HD22	1.81	0.46
1:A:128:TRP:CG	1:A:129:PRO:HD3	2.50	0.46
3:C:206:ARG:NH1	3:C:262:SER:O	2.48	0.46
3:M:167:TRP:NE1	3:M:182:ARG:HG2	2.30	0.46
3:I:266:GLN:CG	11:I:323:FC6:C22	2.93	0.46
3:I:130:GLN:HE21	3:I:130:GLN:CA	2.24	0.46
3:F:266:GLN:HG2	11:F:323:FC6:C23	2.45	0.46
2:L:57:ARG:NH1	2:L:99:LEU:HD12	2.30	0.46
1:G:372:ARG:HH11	1:G:372:ARG:HB2	1.80	0.46
3:M:212:LEU:HD23	3:M:212:LEU:HA	1.66	0.46
1:K:202:GLN:O	1:K:206:GLY:N	2.44	0.45
1:A:218:PHE:CD2	1:A:221:ILE:HD12	2.52	0.45
3:M:74:VAL:O	3:M:82:TRP:HZ3	1.98	0.45
1:A:125:GLU:HG2	1:A:125:GLU:H	1.39	0.45
1:G:90:PHE:CD1	1:G:147:GLY:HA3	2.51	0.45
3:I:167:TRP:NE1	3:I:182:ARG:HG2	2.32	0.45
1:K:335:LEU:HD13	4:Z:707:UNK:HA	1.98	0.45
2:B:129:ARG:CZ	2:B:129:ARG:HB2	2.46	0.45
1:D:413:ILE:HG22	1:D:414:ASN:O	2.16	0.45
2:B:47:LYS:HE2	3:I:221:ASP:OD2	2.16	0.45
3:M:121:SER:O	3:M:125:VAL:HG23	2.16	0.45
1:K:57:ARG:NH1	5:K:502:HEM:O2A	2.50	0.45
2:B:63:GLU:HA	2:B:63:GLU:OE1	2.16	0.45
1:D:125:GLU:H	1:D:125:GLU:HG2	1.44	0.45
1:D:226:VAL:HB	1:D:227:PRO:HD3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:250:VAL:HG11	1:G:278:ILE:HG22	1.99	0.45
1:D:218:PHE:CD2	1:D:221:ILE:HD12	2.52	0.45
1:K:346:VAL:HG22	5:K:501:HEM:C3D	2.52	0.45
1:K:61:THR:HG22	1:K:62:ASN:ND2	2.28	0.45
1:G:339:THR:HG22	1:G:410:TRP:CZ3	2.52	0.45
4:U:715:UNK:C	4:U:717:UNK:N	2.79	0.45
1:K:60:HIS:O	1:K:64:VAL:HB	2.17	0.45
3:C:229:TYR:CD2	3:C:233:CYS:HB2	2.52	0.45
1:K:227:PRO:HB2	3:M:47:ILE:CD1	2.45	0.45
1:D:209:ALA:O	1:D:213:PHE:CB	2.64	0.45
11:C:323:FC6:N25	3:M:215:PRO:HG3	2.30	0.45
3:F:167:TRP:NE1	3:F:182:ARG:HG2	2.31	0.45
1:A:58:PRO:HA	1:A:61:THR:HB	1.97	0.45
1:G:58:PRO:HA	1:G:61:THR:HB	1.99	0.45
3:M:130:GLN:NE2	3:M:130:GLN:HA	2.30	0.45
3:C:37:ASP:HB3	3:C:38:GLN:H	1.65	0.45
1:A:367:PRO:HD3	1:A:375:MET:HE3	1.99	0.45
1:D:13:VAL:HA	1:D:16:GLN:NE2	2.32	0.45
3:M:167:TRP:CD2	3:M:182:ARG:HG2	2.50	0.45
1:G:413:ILE:HG22	1:G:414:ASN:O	2.17	0.45
3:M:282:GLN:HG3	10:M:322:HEC:HBB2	1.98	0.45
1:D:200:MET:HG3	1:D:264:LEU:HD11	1.98	0.45
2:H:48:PRO:HG3	2:H:166:PRO:HD2	1.98	0.45
3:I:85:VAL:O	3:I:85:VAL:CG1	2.64	0.45
1:K:410:TRP:O	2:L:82:ARG:NH1	2.50	0.45
1:G:55:ARG:NH2	2:H:62:ARG:HD2	2.32	0.45
1:A:319:MET:HG3	1:A:320:SER:N	2.29	0.45
3:M:189:TRP:O	3:M:193:ILE:HG22	2.17	0.44
1:G:308:ARG:NH1	1:G:382:ASN:HD21	2.15	0.44
3:F:237:HIS:HE1	3:F:250:PRO:HD2	1.82	0.44
1:A:376:HIS:CB	1:A:458:THR:HG22	2.46	0.44
3:I:121:SER:O	3:I:125:VAL:HG23	2.17	0.44
1:D:202:GLN:O	1:D:206:GLY:N	2.44	0.44
3:F:179:LEU:HD23	3:F:291:VAL:HG11	1.98	0.44
3:M:302:SER:O	3:M:303:GLN:HB3	2.16	0.44
3:C:85:VAL:CG1	3:C:85:VAL:O	2.64	0.44
1:G:402:ASN:OD1	1:G:433:GLY:HA3	2.17	0.44
1:A:94:LEU:O	1:A:98:THR:HG23	2.18	0.44
2:L:157:MET:CE	2:L:171:ASP:HB3	2.39	0.44
1:D:58:PRO:HA	1:D:61:THR:HB	1.99	0.44
1:G:340:ASP:H	1:G:406:GLN:HE22	1.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:212:LEU:HD23	3:C:212:LEU:HA	1.69	0.44
1:A:324:GLY:HA3	5:A:501:HEM:C1B	2.52	0.44
2:B:137:MET:HG3	10:B:211:HEC:NC	2.33	0.44
1:K:376:HIS:HB2	1:K:458:THR:HG22	2.00	0.44
1:D:376:HIS:CB	1:D:458:THR:HG22	2.48	0.44
3:C:187:PRO:HG2	3:C:189:TRP:CZ2	2.52	0.44
3:I:130:GLN:HA	3:I:130:GLN:NE2	2.31	0.44
3:F:130:GLN:HE21	3:F:130:GLN:CA	2.28	0.44
1:K:367:PRO:HG3	1:K:375:MET:HE2	1.99	0.44
1:D:174:LEU:HD12	1:D:204:TRP:CZ2	2.52	0.44
3:C:240:GLY:C	3:C:242:GLU:OE1	2.55	0.44
3:M:255:ALA:HA	3:M:258:TRP:CD2	2.53	0.44
3:F:264:LEU:HB2	11:I:323:FC6:N25	2.32	0.44
1:D:342:THR:O	1:D:346:VAL:HG23	2.17	0.44
1:K:94:LEU:O	1:K:98:THR:HG23	2.17	0.44
11:F:323:FC6:N25	3:I:215:PRO:HG3	2.33	0.44
1:D:235:TYR:O	1:D:289:ASN:ND2	2.51	0.44
1:G:346:VAL:HG22	5:G:501:HEM:C3D	2.51	0.44
3:F:229:TYR:CD2	3:F:233:CYS:HB2	2.52	0.44
2:B:157:MET:HE2	2:B:172:ILE:HA	1.99	0.44
1:G:64:VAL:O	1:G:68:PHE:HB3	2.18	0.44
1:G:200:MET:HG3	1:G:264:LEU:HD11	2.00	0.44
1:D:94:LEU:O	1:D:98:THR:HG23	2.17	0.44
1:K:260:HIS:HB2	1:K:333:ASN:OD1	2.18	0.44
3:I:189:TRP:CZ3	3:I:232:THR:HG21	2.52	0.44
1:K:64:VAL:O	1:K:68:PHE:HB3	2.18	0.44
2:H:137:MET:HB2	10:H:211:HEC:C1D	2.48	0.44
1:D:377:SER:H	1:D:454:ASN:HD21	1.65	0.44
1:D:115:LEU:HB3	1:D:117:PHE:CE2	2.52	0.44
1:G:66:PHE:O	1:G:70:GLY:HA3	2.18	0.44
1:D:196:ALA:HB3	2:E:39:VAL:HB	1.98	0.44
1:K:218:PHE:HA	1:K:221:ILE:HG13	1.99	0.43
1:G:57:ARG:NH1	5:G:502:HEM:O2A	2.51	0.43
1:G:209:ALA:O	1:G:213:PHE:CB	2.66	0.43
1:G:327:MET:HB2	1:G:327:MET:HE2	1.79	0.43
3:M:163:GLN:HA	3:M:163:GLN:HE21	1.81	0.43
3:F:282:GLN:HG3	10:F:322:HEC:HBB2	2.00	0.43
1:D:372:ARG:CZ	1:D:461:ALA:HB1	2.48	0.43
1:G:376:HIS:HB2	1:G:458:THR:HG22	2.00	0.43
1:K:13:VAL:HA	1:K:16:GLN:NE2	2.31	0.43
3:M:179:LEU:HD22	3:M:283:GLN:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:260:HIS:HB2	1:D:333:ASN:OD1	2.17	0.43
2:B:127:ASN:HD22	2:B:127:ASN:C	2.21	0.43
1:K:359:ILE:CD1	1:K:448:MET:HE1	2.15	0.43
5:G:502:HEM:HBB2	5:G:502:HEM:CHC	2.34	0.43
1:G:218:PHE:CD2	1:G:221:ILE:HD12	2.54	0.43
1:K:460:GLN:O	1:K:461:ALA:C	2.57	0.43
1:G:267:TRP:HE1	2:H:36:GLN:HE22	1.65	0.43
1:G:196:ALA:HB3	2:H:39:VAL:HB	2.00	0.43
1:G:310:LEU:O	1:G:313:SER:HB3	2.18	0.43
3:C:130:GLN:NE2	3:C:130:GLN:HA	2.33	0.43
1:A:372:ARG:CZ	1:A:461:ALA:HB1	2.48	0.43
1:K:226:VAL:HB	1:K:227:PRO:HD3	2.00	0.43
3:F:271:ILE:CG1	10:F:321:HEC:HMB2	2.44	0.43
3:C:189:TRP:CH2	3:C:232:THR:CG2	3.02	0.43
5:D:502:HEM:HHC	5:D:502:HEM:CBB	2.36	0.43
1:A:372:ARG:HH11	1:A:372:ARG:HB2	1.83	0.43
1:D:227:PRO:HB2	3:F:47:ILE:CD1	2.48	0.43
1:A:267:TRP:HE1	2:B:36:GLN:HE22	1.65	0.43
1:A:260:HIS:HB2	1:A:333:ASN:OD1	2.18	0.43
1:D:182:ILE:HD12	2:E:163:LEU:HG	2.01	0.43
1:K:264:LEU:HD12	1:K:265:PRO:HD2	1.99	0.43
1:G:239:LEU:HD23	1:G:289:ASN:ND2	2.33	0.43
3:I:47:ILE:HG12	3:I:47:ILE:H	1.62	0.43
11:C:323:FC6:C21	3:M:215:PRO:HG3	2.48	0.43
10:C:321:HEC:HBC2	10:C:321:HEC:HHH	2.00	0.43
2:E:116:TYR:CE2	3:F:145:ILE:CG2	2.95	0.43
2:H:36:GLN:O	2:H:40:ASN:ND2	2.51	0.43
1:D:308:ARG:NH1	1:D:382:ASN:HD21	2.17	0.43
1:G:195:GLY:HA2	2:H:92:SER:HB2	2.00	0.43
1:A:305:PRO:HB3	1:A:382:ASN:HD22	1.83	0.43
3:M:117:TYR:CE1	3:M:131:ALA:HB2	2.54	0.43
1:A:351:LEU:O	1:A:355:ALA:HB3	2.19	0.43
1:K:64:VAL:HG21	5:K:502:HEM:C2C	2.53	0.43
1:D:356:MET:CE	1:D:388:ALA:CB	2.96	0.43
1:K:61:THR:HG22	1:K:62:ASN:N	2.34	0.43
2:B:116:TYR:HE2	3:C:145:ILE:CG2	2.28	0.43
1:K:66:PHE:O	1:K:70:GLY:HA3	2.18	0.43
1:A:295:SER:HA	1:A:298:TRP:NE1	2.34	0.43
1:A:152:ARG:HH12	2:B:11:VAL:CG2	2.32	0.43
3:I:37:ASP:HB3	3:I:38:GLN:H	1.69	0.43
1:D:305:PRO:HB3	1:D:382:ASN:HD22	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:ILE:HG22	1:A:414:ASN:O	2.19	0.43
3:C:255:ALA:HA	3:C:258:TRP:CD2	2.54	0.43
1:D:256:PRO:HB2	1:D:272:GLY:HA3	2.00	0.43
3:F:269:GLN:HG2	11:F:323:FC6:N24	2.34	0.42
2:H:124:HIS:HE1	10:H:211:HEC:C1A	2.32	0.42
1:A:227:PRO:HB2	3:C:47:ILE:HD12	2.01	0.42
1:D:108:LEU:HA	1:D:108:LEU:HD12	1.93	0.42
1:A:193:TYR:CE1	1:A:201:VAL:HG11	2.54	0.42
3:C:157:PHE:HA	3:C:158:PRO:HD3	1.79	0.42
2:H:189:VAL:O	2:H:193:GLN:HG2	2.19	0.42
1:A:64:VAL:O	1:A:68:PHE:HB3	2.19	0.42
1:G:64:VAL:HG21	5:G:502:HEM:C2C	2.54	0.42
1:K:62:ASN:HD21	1:K:125:GLU:HG3	1.83	0.42
2:H:129:ARG:HD3	2:H:135:SER:O	2.19	0.42
3:F:130:GLN:HA	3:F:130:GLN:NE2	2.34	0.42
1:D:128:TRP:CG	1:D:129:PRO:HD3	2.55	0.42
4:Z:720:UNK:C	4:Z:722:UNK:H	2.33	0.42
4:U:713:UNK:O	4:U:714:UNK:C	2.66	0.42
2:L:127:ASN:C	2:L:127:ASN:ND2	2.73	0.42
1:D:60:HIS:O	1:D:64:VAL:HB	2.19	0.42
1:G:61:THR:HG22	1:G:62:ASN:N	2.34	0.42
3:F:47:ILE:HG12	3:F:47:ILE:H	1.62	0.42
1:G:13:VAL:HA	1:G:16:GLN:NE2	2.34	0.42
1:D:193:TYR:CE1	1:D:201:VAL:HG11	2.54	0.42
1:D:267:TRP:HE1	2:E:36:GLN:HE22	1.67	0.42
1:K:200:MET:HG3	1:K:264:LEU:HD11	2.01	0.42
3:F:209:LEU:O	3:F:253:ASN:HA	2.20	0.42
1:G:60:HIS:O	1:G:64:VAL:HB	2.18	0.42
2:B:140:TYR:CE1	10:B:211:HEC:HBB2	2.54	0.42
1:A:84:THR:HG21	1:A:161:ASN:HD21	1.84	0.42
1:G:227:PRO:HB2	3:I:47:ILE:CD1	2.50	0.42
1:G:256:PRO:HB2	1:G:272:GLY:HA3	2.00	0.42
3:C:221:ASP:OD2	2:H:47:LYS:HE2	2.19	0.42
4:Y:728:UNK:C	4:Y:730:UNK:N	2.83	0.42
2:H:183:THR:O	2:H:186:ASP:HB2	2.19	0.42
1:A:379:GLY:O	1:A:383:THR:HG23	2.20	0.42
1:G:294:LEU:HD22	1:G:311:VAL:HG21	2.01	0.42
3:F:189:TRP:CD1	10:F:321:HEC:HBB2	2.55	0.42
1:A:356:MET:CE	1:A:388:ALA:CB	2.97	0.42
3:F:99:TRP:O	3:F:103:VAL:HG23	2.19	0.42
3:C:240:GLY:HA3	3:C:242:GLU:OE1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:15:ARG:HG2	1:K:370:PHE:CZ	2.55	0.42
1:A:159:VAL:HA	1:A:162:TRP:CD2	2.55	0.42
3:C:152:LYS:O	3:C:159:ASN:HB2	2.19	0.42
3:F:121:SER:O	3:F:125:VAL:HG23	2.19	0.42
1:D:252:ILE:HD11	2:E:22:VAL:HG22	2.02	0.42
1:D:218:PHE:HA	1:D:221:ILE:HG13	2.02	0.42
3:F:277:GLY:HA3	10:F:322:HEC:O1D	2.19	0.42
1:G:325:PRO:CD	5:G:501:HEM:HBB2	2.44	0.42
2:B:25:GLY:HA2	2:B:28:THR:HG22	2.02	0.42
1:D:22:VAL:O	1:D:26:ILE:HG12	2.19	0.42
2:E:48:PRO:HG3	2:E:166:PRO:HD2	2.02	0.42
4:U:720:UNK:C	4:U:722:UNK:N	2.83	0.42
3:M:37:ASP:HB3	3:M:38:GLN:H	1.68	0.42
2:L:127:ASN:HD22	2:L:127:ASN:C	2.23	0.42
1:G:199:ALA:HA	2:H:98:PHE:CZ	2.54	0.42
1:G:359:ILE:HD12	1:G:384:HIS:HE1	1.85	0.42
3:F:224:ALA:O	3:F:228:VAL:HG23	2.19	0.42
1:A:239:LEU:HD23	1:A:289:ASN:ND2	2.33	0.42
3:I:241:GLY:N	3:I:242:GLU:OE1	2.53	0.42
1:A:376:HIS:HB2	1:A:458:THR:HG22	2.01	0.42
1:A:128:TRP:CE2	1:A:183:PRO:HB3	2.55	0.42
3:F:85:VAL:O	3:F:85:VAL:CG1	2.68	0.42
3:F:157:PHE:HA	3:F:158:PRO:HD3	1.81	0.42
1:D:76:THR:CG2	1:D:221:ILE:HG12	2.36	0.41
3:C:167:TRP:NE1	3:C:182:ARG:HG2	2.34	0.41
1:K:356:MET:CE	1:K:388:ALA:CB	2.98	0.41
2:L:183:THR:O	2:L:186:ASP:HB2	2.19	0.41
3:F:24:ILE:HD12	3:F:59:PHE:CD2	2.55	0.41
2:H:43:VAL:O	2:H:46:MET:HB3	2.19	0.41
1:G:170:THR:HG21	1:G:212:PHE:CE2	2.54	0.41
1:G:335:LEU:CD2	4:Y:710:UNK:CB	2.92	0.41
2:L:120:TRP:NE1	2:L:131:VAL:HG11	2.35	0.41
3:C:179:LEU:HD22	3:C:283:GLN:HB2	2.02	0.41
2:B:129:ARG:O	2:B:133:PRO:HA	2.20	0.41
2:H:125:LEU:HD21	10:H:211:HEC:HMB2	2.01	0.41
2:E:80:THR:HA	2:E:84:GLY:O	2.19	0.41
3:C:47:ILE:H	3:C:47:ILE:HG12	1.60	0.41
2:E:109:LEU:O	2:E:112:VAL:HG22	2.20	0.41
1:G:56:LEU:HD23	1:G:56:LEU:HA	1.90	0.41
3:F:212:LEU:HA	3:F:212:LEU:HD23	1.86	0.41
3:I:89:TYR:HA	3:I:101:ARG:HH12	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:287:MET:HG3	1:D:288:ILE:N	2.35	0.41
1:D:243:HIS:HD2	1:D:282:PRO:O	2.03	0.41
1:K:237:TYR:CZ	1:K:241:ILE:HD11	2.56	0.41
3:C:240:GLY:CA	3:C:242:GLU:OE1	2.68	0.41
2:H:72:MET:HE2	2:H:100:TRP:CD2	2.56	0.41
1:D:319:MET:HG3	1:D:320:SER:N	2.31	0.41
1:A:287:MET:HG3	1:A:288:ILE:N	2.35	0.41
3:I:255:ALA:HA	3:I:258:TRP:CD2	2.55	0.41
2:H:127:ASN:C	2:H:127:ASN:HD22	2.24	0.41
3:M:130:GLN:HE21	3:M:130:GLN:CA	2.23	0.41
1:K:454:ASN:O	1:K:458:THR:CG2	2.66	0.41
3:F:250:PRO:HG3	10:F:321:HEC:HBA1	2.02	0.41
3:M:47:ILE:HG12	3:M:47:ILE:H	1.62	0.41
1:A:376:HIS:HB3	1:A:454:ASN:ND2	2.35	0.41
1:G:110:ALA:O	1:G:114:PRO:HD2	2.21	0.41
1:A:29:MET:SD	1:A:448:MET:HG3	2.60	0.41
1:K:55:ARG:NH2	2:L:62:ARG:HD2	2.35	0.41
1:D:84:THR:HG21	1:D:161:ASN:HD21	1.85	0.41
1:A:174:LEU:HD12	1:A:204:TRP:CZ2	2.56	0.41
1:G:414:ASN:HD21	1:G:420:THR:HG23	1.86	0.41
3:M:85:VAL:CG1	3:M:85:VAL:O	2.69	0.41
1:G:319:MET:HG3	1:G:320:SER:N	2.32	0.41
1:D:199:ALA:HA	2:E:98:PHE:CZ	2.55	0.41
10:F:321:HEC:HBC2	10:F:321:HEC:HHD	2.03	0.41
1:D:170:THR:HB	2:E:22:VAL:HG21	2.03	0.41
1:A:218:PHE:HA	1:A:221:ILE:HG13	2.02	0.41
1:D:64:VAL:HG11	5:D:502:HEM:CHD	2.51	0.41
1:G:324:GLY:HA3	5:G:501:HEM:C1B	2.55	0.41
1:K:324:GLY:HA3	5:K:501:HEM:C1B	2.56	0.41
2:L:137:MET:HB2	10:L:211:HEC:C1D	2.51	0.41
3:C:179:LEU:HD23	3:C:291:VAL:HG11	2.02	0.41
2:E:43:VAL:O	2:E:46:MET:HB3	2.21	0.41
1:G:159:VAL:HA	1:G:162:TRP:CD2	2.55	0.41
1:A:64:VAL:HG21	5:A:502:HEM:C2C	2.55	0.41
1:D:57:ARG:NH1	5:D:502:HEM:O2A	2.54	0.41
1:K:243:HIS:HD2	1:K:282:PRO:O	2.03	0.41
1:K:281:ALA:CB	1:K:282:PRO:HD3	2.42	0.41
3:F:239:GLN:N	3:F:239:GLN:OE1	2.49	0.41
1:A:84:THR:HG21	1:A:161:ASN:ND2	2.35	0.41
1:K:209:ALA:O	1:K:213:PHE:HB3	2.21	0.41
2:B:152:ASP:HA	2:B:155:LYS:HE3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:GLN:NE2	3:C:95:GLN:HE22	2.19	0.41
4:Z:726:UNK:C	4:Z:728:UNK:N	2.82	0.41
1:K:305:PRO:HB3	1:K:382:ASN:HD22	1.86	0.41
2:H:74:ARG:HA	2:H:75:PRO:HD3	1.86	0.41
3:C:74:VAL:O	3:C:82:TRP:HZ3	2.01	0.41
1:D:242:VAL:HG13	3:F:23:LEU:HD13	2.03	0.41
1:K:305:PRO:O	1:K:308:ARG:HB2	2.20	0.41
2:H:80:THR:HA	2:H:84:GLY:O	2.21	0.41
3:I:166:ARG:NH2	3:I:250:PRO:HG3	2.36	0.41
3:I:212:LEU:HA	3:I:212:LEU:HD23	1.84	0.41
1:D:376:HIS:HB2	1:D:458:THR:HG22	2.03	0.40
1:A:22:VAL:O	1:A:26:ILE:HG12	2.21	0.40
2:E:88:VAL:HG12	2:E:90:GLY:H	1.86	0.40
3:M:89:TYR:CD1	3:M:101:ARG:NH1	2.88	0.40
3:F:271:ILE:CD1	10:F:321:HEC:HMB2	2.51	0.40
2:E:157:MET:CE	2:E:171:ASP:HB3	2.39	0.40
2:B:43:VAL:O	2:B:44:GLU:C	2.59	0.40
1:D:301:LEU:HD21	1:D:311:VAL:HG21	2.04	0.40
2:E:127:ASN:HD22	2:E:127:ASN:C	2.25	0.40
1:G:108:LEU:HA	1:G:108:LEU:HD12	1.90	0.40
2:H:157:MET:CE	2:H:171:ASP:HB3	2.36	0.40
1:G:349:GLY:O	1:G:353:TRP:HB3	2.22	0.40
1:G:285:GLY:O	1:G:289:ASN:HB2	2.22	0.40
3:M:157:PHE:HA	3:M:158:PRO:HD3	1.83	0.40
3:I:117:TYR:CE1	3:I:131:ALA:HB2	2.56	0.40
3:F:163:GLN:HA	3:F:163:GLN:HE21	1.86	0.40
3:M:79:LEU:O	3:M:82:TRP:HB2	2.20	0.40
2:B:36:GLN:HE21	2:B:36:GLN:HB2	1.75	0.40
1:G:260:HIS:HB2	1:G:333:ASN:OD1	2.21	0.40
3:C:75:LEU:HD22	3:C:86:LEU:HD12	2.03	0.40
1:A:56:LEU:HA	1:A:56:LEU:HD23	1.76	0.40
1:D:218:PHE:CZ	1:D:354:VAL:HG13	2.57	0.40
1:G:458:THR:O	1:G:461:ALA:CB	2.70	0.40
1:D:84:THR:HG21	1:D:161:ASN:ND2	2.36	0.40
3:I:237:HIS:HE1	3:I:250:PRO:HD2	1.87	0.40
1:D:310:LEU:O	1:D:313:SER:HB3	2.21	0.40
2:H:148:LEU:HD11	2:H:187:ALA:HB2	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:34:GLY:CA	3:I:39:THR:OG1[1_556]	2.10	0.10

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%)	432 (93%)	27 (6%)	5 (1%)	17	62
1	D	461/474 (97%)	430 (93%)	26 (6%)	5 (1%)	17	62
1	G	463/474 (98%)	428 (92%)	30 (6%)	5 (1%)	17	62
1	K	463/474 (98%)	430 (93%)	28 (6%)	5 (1%)	17	62
2	B	195/203 (96%)	185 (95%)	8 (4%)	2 (1%)	19	65
2	E	195/203 (96%)	186 (95%)	7 (4%)	2 (1%)	19	65
2	H	195/203 (96%)	184 (94%)	9 (5%)	2 (1%)	19	65
2	L	195/203 (96%)	185 (95%)	8 (4%)	2 (1%)	19	65
3	C	301/311 (97%)	276 (92%)	17 (6%)	8 (3%)	6	39
3	F	301/311 (97%)	276 (92%)	19 (6%)	6 (2%)	9	48
3	I	301/311 (97%)	276 (92%)	19 (6%)	6 (2%)	9	48
3	M	301/311 (97%)	274 (91%)	20 (7%)	7 (2%)	8	44
All	All	3835/3952 (97%)	3562 (93%)	218 (6%)	55 (1%)	14	57

All (55) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	461	ALA
1	A	465	ALA
2	B	44	GLU
3	C	29	LYS
3	C	33	ALA
3	C	37	ASP
1	D	461	ALA

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Mol	Chain	Res	Type
1	D	465	ALA
2	E	44	GLU
3	F	29	LYS
3	F	33	ALA
3	F	37	ASP
1	G	461	ALA
1	G	465	ALA
2	H	44	GLU
3	I	29	LYS
3	I	33	ALA
3	I	37	ASP
1	K	461	ALA
1	K	465	ALA
2	L	44	GLU
3	M	29	LYS
3	M	33	ALA
3	M	37	ASP
3	C	36	THR
3	C	82	TRP
3	F	36	THR
3	F	82	TRP
3	I	36	THR
3	I	82	TRP
3	M	36	THR
3	M	82	TRP
3	M	190	GLY
2	B	7	LEU
1	D	236	SER
2	E	7	LEU
1	G	236	SER
2	H	7	LEU
1	K	236	SER
2	L	7	LEU
3	C	42	HIS
3	F	42	HIS
3	I	42	HIS
3	M	42	HIS
1	A	236	SER
3	C	301	LEU
1	D	466	GLU
1	G	466	GLU
1	K	466	GLU

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Mol	Chain	Res	Type
1	A	463	LYS
1	A	466	GLU
1	D	463	LYS
1	G	463	LYS
1	K	463	LYS
3	C	238	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	374/379 (99%)	331 (88%)	43 (12%)	7	30
1	D	371/379 (98%)	328 (88%)	43 (12%)	7	30
1	G	373/379 (98%)	327 (88%)	46 (12%)	6	27
1	K	373/379 (98%)	330 (88%)	43 (12%)	7	30
2	B	166/172 (96%)	148 (89%)	18 (11%)	8	33
2	E	166/172 (96%)	148 (89%)	18 (11%)	8	33
2	H	166/172 (96%)	148 (89%)	18 (11%)	8	33
2	L	166/172 (96%)	148 (89%)	18 (11%)	8	33
3	C	227/234 (97%)	203 (89%)	24 (11%)	8	34
3	F	227/234 (97%)	200 (88%)	27 (12%)	6	28
3	I	227/234 (97%)	202 (89%)	25 (11%)	8	33
3	M	227/234 (97%)	200 (88%)	27 (12%)	6	28
All	All	3063/3140 (98%)	2713 (89%)	350 (11%)	7	31

All (350) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	LEU
1	A	50	TRP
1	A	57	ARG
1	A	59	LEU

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Mol	Chain	Res	Type
1	A	61	THR
1	A	64	VAL
1	A	73	LEU
1	A	84	THR
1	A	87	THR
1	A	104	LEU
1	A	107	LEU
1	A	108	LEU
1	A	115	LEU
1	A	118	THR
1	A	120	SER
1	A	125	GLU
1	A	154	VAL
1	A	159	VAL
1	A	167	PHE
1	A	170	THR
1	A	174	LEU
1	A	192	LEU
1	A	200	MET
1	A	210	VAL
1	A	243	HIS
1	A	248	ILE
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	302	ARG
1	A	313	SER
1	A	319	MET
1	A	336	SER
1	A	357	VAL
1	A	372	ARG
1	A	373	GLU
1	A	395	TYR
1	A	427	LEU
1	A	454	ASN
1	A	458	THR
2	B	7	LEU
2	B	13	LEU
2	B	16	LEU

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Mol	Chain	Res	Type
2	B	22	VAL
2	B	27	LEU
2	B	54	LEU
2	B	62	ARG
2	B	66	VAL
2	B	92	SER
2	B	112	VAL
2	B	115	ARG
2	B	127	ASN
2	B	129	ARG
2	B	134	GLU
2	B	177	ASP
2	B	178	SER
2	B	193	GLN
2	B	194	VAL
3	C	3	THR
3	C	11	LEU
3	C	23	LEU
3	C	24	ILE
3	C	35	THR
3	C	39	THR
3	C	56	ARG
3	C	62	PHE
3	C	71	LEU
3	C	82	TRP
3	C	83	LYS
3	C	100	GLU
3	C	130	GLN
3	C	145	ILE
3	C	163	GLN
3	C	175	LYS
3	C	179	LEU
3	C	182	ARG
3	C	186	MET
3	C	193	ILE
3	C	201	VAL
3	C	251	LYS
3	C	264	LEU
3	C	301	LEU
1	D	48	LEU
1	D	50	TRP
1	D	57	ARG

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Mol	Chain	Res	Type
1	D	59	LEU
1	D	61	THR
1	D	64	VAL
1	D	73	LEU
1	D	84	THR
1	D	87	THR
1	D	104	LEU
1	D	107	LEU
1	D	108	LEU
1	D	115	LEU
1	D	118	THR
1	D	120	SER
1	D	125	GLU
1	D	154	VAL
1	D	159	VAL
1	D	167	PHE
1	D	170	THR
1	D	174	LEU
1	D	192	LEU
1	D	200	MET
1	D	210	VAL
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	287	MET
1	D	289	ASN
1	D	294	LEU
1	D	313	SER
1	D	319	MET
1	D	336	SER
1	D	357	VAL
1	D	372	ARG
1	D	373	GLU
1	D	395	TYR
1	D	427	LEU
1	D	454	ASN
1	D	458	THR
2	E	7	LEU
2	E	13	LEU

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Mol	Chain	Res	Type
2	E	16	LEU
2	E	22	VAL
2	E	27	LEU
2	E	54	LEU
2	E	62	ARG
2	E	66	VAL
2	E	92	SER
2	E	112	VAL
2	E	115	ARG
2	E	127	ASN
2	E	129	ARG
2	E	134	GLU
2	E	177	ASP
2	E	178	SER
2	E	193	GLN
2	E	194	VAL
3	F	1	MET
3	F	3	THR
3	F	11	LEU
3	F	23	LEU
3	F	24	ILE
3	F	35	THR
3	F	39	THR
3	F	56	ARG
3	F	62	PHE
3	F	71	LEU
3	F	82	TRP
3	F	83	LYS
3	F	85	VAL
3	F	100	GLU
3	F	130	GLN
3	F	145	ILE
3	F	163	GLN
3	F	175	LYS
3	F	179	LEU
3	F	182	ARG
3	F	186	MET
3	F	193	ILE
3	F	201	VAL
3	F	251	LYS
3	F	264	LEU
3	F	301	LEU

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Mol	Chain	Res	Type
3	F	302	SER
1	G	6	SER
1	G	10	SER
1	G	48	LEU
1	G	50	TRP
1	G	57	ARG
1	G	59	LEU
1	G	61	THR
1	G	64	VAL
1	G	73	LEU
1	G	84	THR
1	G	87	THR
1	G	104	LEU
1	G	107	LEU
1	G	108	LEU
1	G	112	SER
1	G	115	LEU
1	G	118	THR
1	G	120	SER
1	G	125	GLU
1	G	154	VAL
1	G	167	PHE
1	G	170	THR
1	G	174	LEU
1	G	192	LEU
1	G	200	MET
1	G	210	VAL
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	287	MET
1	G	289	ASN
1	G	294	LEU
1	G	302	ARG
1	G	313	SER
1	G	319	MET
1	G	336	SER
1	G	357	VAL
1	G	358	SER

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Mol	Chain	Res	Type
1	G	372	ARG
1	G	373	GLU
1	G	427	LEU
1	G	454	ASN
1	G	458	THR
2	H	7	LEU
2	H	13	LEU
2	H	16	LEU
2	H	22	VAL
2	H	27	LEU
2	H	54	LEU
2	H	62	ARG
2	H	66	VAL
2	H	92	SER
2	H	112	VAL
2	H	115	ARG
2	H	127	ASN
2	H	129	ARG
2	H	134	GLU
2	H	177	ASP
2	H	178	SER
2	H	193	GLN
2	H	194	VAL
3	I	11	LEU
3	I	23	LEU
3	I	24	ILE
3	I	35	THR
3	I	39	THR
3	I	54	LEU
3	I	56	ARG
3	I	62	PHE
3	I	71	LEU
3	I	82	TRP
3	I	83	LYS
3	I	85	VAL
3	I	100	GLU
3	I	130	GLN
3	I	145	ILE
3	I	163	GLN
3	I	175	LYS
3	I	179	LEU
3	I	182	ARG

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Mol	Chain	Res	Type
3	I	186	MET
3	I	193	ILE
3	I	201	VAL
3	I	251	LYS
3	I	264	LEU
3	I	301	LEU
1	K	48	LEU
1	K	50	TRP
1	K	57	ARG
1	K	59	LEU
1	K	61	THR
1	K	64	VAL
1	K	73	LEU
1	K	84	THR
1	K	87	THR
1	K	104	LEU
1	K	107	LEU
1	K	108	LEU
1	K	115	LEU
1	K	118	THR
1	K	120	SER
1	K	125	GLU
1	K	154	VAL
1	K	159	VAL
1	K	167	PHE
1	K	170	THR
1	K	174	LEU
1	K	192	LEU
1	K	193	TYR
1	K	200	MET
1	K	210	VAL
1	K	243	HIS
1	K	248	ILE
1	K	251	TYR
1	K	271	LEU
1	K	275	MET
1	K	278	ILE
1	K	287	MET
1	K	289	ASN
1	K	294	LEU
1	K	313	SER
1	K	319	MET

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Mol	Chain	Res	Type
1	K	336	SER
1	K	357	VAL
1	K	372	ARG
1	K	373	GLU
1	K	427	LEU
1	K	454	ASN
1	K	458	THR
2	L	7	LEU
2	L	13	LEU
2	L	16	LEU
2	L	22	VAL
2	L	27	LEU
2	L	54	LEU
2	L	62	ARG
2	L	66	VAL
2	L	92	SER
2	L	112	VAL
2	L	115	ARG
2	L	127	ASN
2	L	129	ARG
2	L	134	GLU
2	L	177	ASP
2	L	178	SER
2	L	193	GLN
2	L	194	VAL
3	M	1	MET
3	M	11	LEU
3	M	23	LEU
3	M	24	ILE
3	M	35	THR
3	M	39	THR
3	M	54	LEU
3	M	56	ARG
3	M	62	PHE
3	M	71	LEU
3	M	82	TRP
3	M	83	LYS
3	M	85	VAL
3	M	100	GLU
3	M	130	GLN
3	M	145	ILE
3	M	163	GLN

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Mol	Chain	Res	Type
3	M	175	LYS
3	M	179	LEU
3	M	182	ARG
3	M	186	MET
3	M	193	ILE
3	M	201	VAL
3	M	251	LYS
3	M	264	LEU
3	M	301	LEU
3	M	302	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (109) 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	175	HIS
1	A	178	ASN
1	A	243	HIS
1	A	269	GLN
1	A	289	ASN
1	A	374	GLN
1	A	382	ASN
1	A	406	GLN
1	A	414	ASN
1	A	431	HIS
1	A	454	ASN
1	A	460	GLN
2	B	10	ASN
2	B	29	GLN
2	B	36	GLN
2	B	127	ASN
2	B	193	GLN
3	C	98	GLN
3	C	105	GLN
3	C	130	GLN
3	C	163	GLN
3	C	231	GLN
3	C	292	HIS

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Mol	Chain	Res	Type
1	D	16	GLN
1	D	62	ASN
1	D	82	GLN
1	D	103	GLN
1	D	161	ASN
1	D	175	HIS
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	454	ASN
1	D	460	GLN
2	E	10	ASN
2	E	29	GLN
2	E	36	GLN
2	E	127	ASN
2	E	193	GLN
3	F	105	GLN
3	F	130	GLN
3	F	163	GLN
3	F	227	ASN
3	F	268	GLN
3	F	292	HIS
1	G	16	GLN
1	G	62	ASN
1	G	82	GLN
1	G	103	GLN
1	G	161	ASN
1	G	175	HIS
1	G	178	ASN
1	G	243	HIS
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

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Mol	Chain	Res	Type
1	G	460	GLN
2	H	10	ASN
2	H	29	GLN
2	H	36	GLN
2	H	127	ASN
2	H	193	GLN
3	I	105	GLN
3	I	130	GLN
3	I	163	GLN
3	I	266	GLN
3	I	268	GLN
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	175	HIS
1	K	178	ASN
1	K	243	HIS
1	K	269	GLN
1	K	289	ASN
1	K	374	GLN
1	K	382	ASN
1	K	406	GLN
1	K	414	ASN
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	127	ASN
2	L	193	GLN
3	M	105	GLN
3	M	130	GLN
3	M	163	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	30,50,50	2.08	4 (13%)	24,82,82	2.48	11 (45%)
5	HEM	A	502	1,7	30,50,50	2.19	6 (20%)	24,82,82	2.59	11 (45%)
9	PO4	A	506	-	4,4,4	0.39	0	6,6,6	0.32	0
8	PEO	A	508	5,6	1,1,1	0.38	0	0,0,0	0.00	-
10	HEC	B	211	2	24,50,50	2.70	3 (12%)	19,82,82	3.25	5 (26%)
10	HEC	C	321	3	24,50,50	2.56	4 (16%)	19,82,82	3.08	6 (31%)
10	HEC	C	322	3	24,50,50	2.46	3 (12%)	19,82,82	3.19	9 (47%)
11	FC6	C	323	-	12,12,12	1.17	1 (8%)	0,21,21	0.00	-
5	HEM	D	501	1,8,7	30,50,50	2.31	8 (26%)	24,82,82	2.31	9 (37%)
5	HEM	D	502	1,7	30,50,50	2.16	9 (30%)	24,82,82	2.54	10 (41%)
9	PO4	D	506	-	4,4,4	0.36	0	6,6,6	0.29	0
8	PEO	D	508	5,6	1,1,1	0.46	0	0,0,0	0.00	-
10	HEC	E	211	2	24,50,50	2.52	3 (12%)	19,82,82	2.84	4 (21%)
10	HEC	F	321	3	24,50,50	2.42	4 (16%)	19,82,82	3.01	7 (36%)
10	HEC	F	322	3	24,50,50	2.51	3 (12%)	19,82,82	2.80	7 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	FC6	F	323	-	12,12,12	0.95	0	0,21,21	0.00	-
5	HEM	G	501	1,8,7	30,50,50	2.20	5 (16%)	24,82,82	2.47	11 (45%)
5	HEM	G	502	1,7	30,50,50	2.25	8 (26%)	24,82,82	2.66	11 (45%)
9	PO4	G	506	-	4,4,4	0.19	0	6,6,6	0.31	0
8	PEO	G	508	5,6	1,1,1	0.57	0	0,0,0	0.00	-
10	HEC	H	211	2	24,50,50	2.57	4 (16%)	19,82,82	3.12	7 (36%)
10	HEC	I	321	3	24,50,50	2.33	4 (16%)	19,82,82	3.20	6 (31%)
10	HEC	I	322	3	24,50,50	2.53	4 (16%)	19,82,82	2.77	8 (42%)
11	FC6	I	323	-	12,12,12	0.94	0	0,21,21	0.00	-
5	HEM	K	501	1,8,7	30,50,50	2.08	6 (20%)	24,82,82	2.36	10 (41%)
5	HEM	K	502	1,7	30,50,50	2.12	7 (23%)	24,82,82	2.48	11 (45%)
9	PO4	K	506	-	4,4,4	0.37	0	6,6,6	0.30	0
8	PEO	K	508	5,6	1,1,1	0.43	0	0,0,0	0.00	-
10	HEC	L	211	2	24,50,50	2.63	3 (12%)	19,82,82	2.95	6 (31%)
10	HEC	M	321	3	24,50,50	2.52	5 (20%)	19,82,82	3.50	7 (36%)
10	HEC	M	322	3	24,50,50	2.54	4 (16%)	19,82,82	2.94	7 (36%)
11	FC6	M	323	-	12,12,12	1.14	2 (16%)	0,21,21	0.00	-

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	-	0/10/54/54	0/0/8/8
5	HEM	A	502	1,7	-	0/10/54/54	0/0/8/8
9	PO4	A	506	-	-	0/0/0/0	0/0/0/0
8	PEO	A	508	5,6	-	0/0/0/0	0/0/0/0
10	HEC	B	211	2	-	0/6/54/54	0/0/8/8
10	HEC	C	321	3	-	0/6/54/54	0/0/8/8
10	HEC	C	322	3	-	0/6/54/54	0/0/8/8
11	FC6	C	323	-	-	0/0/30/30	0/0/0/0
5	HEM	D	501	1,8,7	-	0/10/54/54	0/0/8/8
5	HEM	D	502	1,7	-	0/10/54/54	0/0/8/8
9	PO4	D	506	-	-	0/0/0/0	0/0/0/0
8	PEO	D	508	5,6	-	0/0/0/0	0/0/0/0
10	HEC	E	211	2	-	0/6/54/54	0/0/8/8
10	HEC	F	321	3	-	0/6/54/54	0/0/8/8
10	HEC	F	322	3	-	0/6/54/54	0/0/8/8
11	FC6	F	323	-	-	0/0/30/30	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	HEM	G	501	1,8,7	-	0/10/54/54	0/0/8/8
5	HEM	G	502	1,7	-	0/10/54/54	0/0/8/8
9	PO4	G	506	-	-	0/0/0/0	0/0/0/0
8	PEO	G	508	5,6	-	0/0/0/0	0/0/0/0
10	HEC	H	211	2	-	0/6/54/54	0/0/8/8
10	HEC	I	321	3	-	0/6/54/54	0/0/8/8
10	HEC	I	322	3	-	0/6/54/54	0/0/8/8
11	FC6	I	323	-	-	0/0/30/30	0/0/0/0
5	HEM	K	501	1,8,7	-	0/10/54/54	0/0/8/8
5	HEM	K	502	1,7	-	0/10/54/54	0/0/8/8
9	PO4	K	506	-	-	0/0/0/0	0/0/0/0
8	PEO	K	508	5,6	-	0/0/0/0	0/0/0/0
10	HEC	L	211	2	-	0/6/54/54	0/0/8/8
10	HEC	M	321	3	-	0/6/54/54	0/0/8/8
10	HEC	M	322	3	-	0/6/54/54	0/0/8/8
11	FC6	M	323	-	-	0/0/30/30	0/0/0/0

All (100) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	211	HEC	C3C-C2C	-8.89	1.31	1.40
10	I	322	HEC	C3C-C2C	-7.92	1.32	1.40
5	G	502	HEM	C3B-C4B	-7.79	1.44	1.51
5	D	501	HEM	C3B-C4B	-7.79	1.44	1.51
10	M	321	HEC	C3C-C2C	-7.78	1.32	1.40
5	G	501	HEM	C3B-C4B	-7.72	1.45	1.51
10	C	321	HEC	C3B-C2B	-7.70	1.32	1.40
10	C	322	HEC	C3C-C2C	-7.66	1.32	1.40
10	L	211	HEC	C3C-C2C	-7.55	1.32	1.40
10	E	211	HEC	C3C-C2C	-7.47	1.32	1.40
5	A	502	HEM	C3B-C4B	-7.42	1.45	1.51
10	H	211	HEC	C3C-C2C	-7.37	1.33	1.40
10	B	211	HEC	C3B-C2B	-7.23	1.33	1.40
10	M	322	HEC	C3C-C2C	-7.19	1.33	1.40
5	A	501	HEM	C3B-C4B	-7.17	1.45	1.51
10	L	211	HEC	C3B-C2B	-7.09	1.33	1.40
10	F	322	HEC	C3C-C2C	-7.00	1.33	1.40
10	M	322	HEC	C3B-C2B	-6.99	1.33	1.40
10	H	211	HEC	C3B-C2B	-6.94	1.33	1.40
10	F	321	HEC	C3B-C2B	-6.89	1.33	1.40
5	D	502	HEM	C3B-C4B	-6.81	1.45	1.51
10	C	322	HEC	C3B-C2B	-6.72	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	I	321	HEC	C3C-C2C	-6.67	1.33	1.40
10	I	322	HEC	C3B-C2B	-6.64	1.33	1.40
10	F	322	HEC	C3B-C2B	-6.59	1.33	1.40
10	E	211	HEC	C3B-C2B	-6.57	1.33	1.40
10	F	321	HEC	C3C-C2C	-6.45	1.34	1.40
10	M	321	HEC	C3B-C2B	-6.41	1.34	1.40
5	K	502	HEM	C3D-C4D	-6.29	1.43	1.51
10	C	321	HEC	C3C-C2C	-6.28	1.34	1.40
5	K	501	HEM	C3B-C4B	-6.01	1.46	1.51
5	K	502	HEM	C3B-C4B	-5.98	1.46	1.51
5	A	502	HEM	C3D-C4D	-5.96	1.43	1.51
5	A	501	HEM	C3D-C4D	-5.80	1.44	1.51
5	K	501	HEM	C3D-C4D	-5.69	1.44	1.51
5	G	502	HEM	C3D-C4D	-5.66	1.44	1.51
10	I	321	HEC	C3B-C2B	-5.46	1.35	1.40
5	G	501	HEM	C3D-C4D	-5.34	1.44	1.51
5	D	502	HEM	C3D-C4D	-5.34	1.44	1.51
5	D	501	HEM	C3D-C4D	-5.19	1.44	1.51
5	G	501	HEM	C2C-C1C	-4.57	1.43	1.52
5	K	501	HEM	C2C-C1C	-4.27	1.44	1.52
5	D	501	HEM	C2C-C1C	-4.00	1.45	1.52
5	D	502	HEM	C2C-C1C	-3.86	1.45	1.52
5	A	501	HEM	C2C-C1C	-3.72	1.45	1.52
5	G	502	HEM	C2C-C1C	-3.65	1.45	1.52
5	K	502	HEM	C2C-C1C	-3.40	1.46	1.52
5	A	502	HEM	C2C-C1C	-3.02	1.46	1.52
11	C	323	FC6	C26-FE2	-2.53	1.85	1.93
5	D	501	HEM	C2D-C1D	-2.40	1.44	1.51
5	A	502	HEM	C2B-C1B	-2.38	1.44	1.51
5	D	502	HEM	C2D-C1D	-2.32	1.44	1.51
5	K	502	HEM	C2B-C1B	-2.26	1.44	1.51
11	M	323	FC6	C22-FE2	-2.21	1.86	1.93
5	K	501	HEM	C2D-C1D	-2.20	1.44	1.51
5	G	502	HEM	C2B-C1B	-2.19	1.44	1.51
5	G	502	HEM	C2D-C1D	-2.19	1.44	1.51
11	M	323	FC6	C23-FE2	-2.16	1.86	1.93
5	K	502	HEM	C2D-C1D	-2.14	1.44	1.51
5	D	502	HEM	C2B-C1B	-2.09	1.45	1.51
5	A	501	HEM	C2D-C1D	-2.09	1.45	1.51
10	M	322	HEC	C2A-C3A	-2.05	1.31	1.37
5	D	502	HEM	C1C-NC	2.01	1.38	1.36
5	D	502	HEM	C3C-CAC	2.05	1.55	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	I	322	HEC	C1A-NA	2.05	1.39	1.36
5	G	502	HEM	C1C-NC	2.06	1.38	1.36
10	M	321	HEC	C4A-NA	2.08	1.39	1.36
10	F	321	HEC	C3C-C4C	2.18	1.47	1.42
5	D	502	HEM	CAA-C2A	2.20	1.55	1.52
5	D	501	HEM	C3B-CAB	2.22	1.55	1.51
5	D	501	HEM	C3C-CAC	2.25	1.55	1.51
5	D	501	HEM	FE-ND	2.27	2.09	1.97
5	G	501	HEM	FE-ND	2.32	2.09	1.97
5	G	502	HEM	CAA-C2A	2.33	1.56	1.52
5	G	502	HEM	FE-NC	2.35	2.05	1.95
10	H	211	HEC	CMA-C3A	2.37	1.56	1.51
5	G	501	HEM	FE-NC	2.39	2.05	1.95
5	K	501	HEM	C3B-CAB	2.41	1.55	1.51
5	K	502	HEM	FE-NB	2.42	2.10	1.97
10	M	321	HEC	C3C-C4C	2.50	1.48	1.42
5	A	502	HEM	FE-NC	2.51	2.05	1.95
10	C	321	HEC	C3C-C4C	2.56	1.48	1.42
10	I	321	HEC	C3C-C4C	2.64	1.48	1.42
5	A	502	HEM	CAA-C2A	2.86	1.56	1.52
5	K	502	HEM	C1C-NC	2.88	1.39	1.36
5	K	501	HEM	FE-NC	2.94	2.07	1.95
5	D	502	HEM	FE-NC	2.97	2.07	1.95
5	D	501	HEM	FE-NC	3.75	2.10	1.95
10	M	321	HEC	C3D-C2D	4.27	1.50	1.37
10	I	322	HEC	C3D-C2D	4.38	1.50	1.37
10	C	322	HEC	C3D-C2D	4.43	1.50	1.37
10	B	211	HEC	C3D-C2D	4.43	1.50	1.37
10	F	321	HEC	C3D-C2D	4.68	1.51	1.37
10	I	321	HEC	C3D-C2D	4.80	1.51	1.37
10	E	211	HEC	C3D-C2D	4.96	1.52	1.37
10	H	211	HEC	C3D-C2D	4.97	1.52	1.37
10	F	322	HEC	C3D-C2D	4.99	1.52	1.37
10	C	321	HEC	C3D-C2D	5.02	1.52	1.37
10	M	322	HEC	C3D-C2D	5.09	1.52	1.37
10	L	211	HEC	C3D-C2D	5.32	1.53	1.37

All (163) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	211	HEC	CBB-CAB-C3B	-10.07	104.97	127.35
10	M	321	HEC	CBB-CAB-C3B	-9.26	106.78	127.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	H	211	HEC	CBB-CAB-C3B	-8.86	107.66	127.35
10	E	211	HEC	CBB-CAB-C3B	-8.39	108.70	127.35
10	L	211	HEC	CBB-CAB-C3B	-8.23	109.06	127.35
10	I	321	HEC	CBB-CAB-C3B	-8.00	109.58	127.35
10	C	321	HEC	CBB-CAB-C3B	-7.62	110.42	127.35
10	C	322	HEC	CBC-CAC-C3C	-7.61	110.44	127.35
10	F	321	HEC	CBB-CAB-C3B	-7.60	110.47	127.35
10	M	321	HEC	CBC-CAC-C3C	-7.39	110.93	127.35
10	C	322	HEC	CBB-CAB-C3B	-7.14	111.48	127.35
10	M	322	HEC	CBB-CAB-C3B	-7.14	111.49	127.35
10	M	322	HEC	CBC-CAC-C3C	-7.00	111.80	127.35
10	F	322	HEC	CBC-CAC-C3C	-6.93	111.96	127.35
10	F	322	HEC	CBB-CAB-C3B	-6.65	112.58	127.35
10	H	211	HEC	CBC-CAC-C3C	-6.62	112.65	127.35
10	B	211	HEC	CBC-CAC-C3C	-6.48	112.95	127.35
10	I	322	HEC	CBB-CAB-C3B	-6.45	113.01	127.35
10	L	211	HEC	CBC-CAC-C3C	-6.35	113.24	127.35
10	E	211	HEC	CBC-CAC-C3C	-6.24	113.48	127.35
10	I	321	HEC	CBC-CAC-C3C	-6.13	113.72	127.35
10	I	321	HEC	CAA-CBA-CGA	-5.97	101.80	112.75
10	F	321	HEC	CAA-CBA-CGA	-5.90	101.94	112.75
10	I	322	HEC	CBC-CAC-C3C	-5.85	114.34	127.35
10	M	321	HEC	CAA-CBA-CGA	-5.81	102.09	112.75
10	C	321	HEC	CBC-CAC-C3C	-5.80	114.46	127.35
10	F	321	HEC	CBC-CAC-C3C	-5.56	114.99	127.35
10	C	321	HEC	CAA-CBA-CGA	-5.52	102.64	112.75
10	M	321	HEC	CBD-CAD-C3D	-5.19	103.23	112.53
10	C	321	HEC	CBD-CAD-C3D	-5.05	103.49	112.53
5	D	502	HEM	CBA-CAA-C2A	-4.81	103.92	112.53
5	G	502	HEM	CBA-CAA-C2A	-4.78	103.96	112.53
10	I	321	HEC	CMC-C2C-C1C	-4.66	120.66	128.36
5	G	501	HEM	CAA-CBA-CGA	-4.59	104.34	112.75
5	K	502	HEM	CBA-CAA-C2A	-4.54	104.38	112.53
10	I	322	HEC	CAD-CBD-CGD	-4.52	104.46	112.75
10	M	322	HEC	CAA-CBA-CGA	-4.37	104.74	112.75
10	I	321	HEC	CBD-CAD-C3D	-4.25	104.92	112.53
10	L	211	HEC	CBA-CAA-C2A	-4.11	105.16	112.53
10	C	321	HEC	CMC-C2C-C1C	-4.10	121.58	128.36
10	H	211	HEC	CBA-CAA-C2A	-4.02	105.32	112.53
10	F	321	HEC	CBD-CAD-C3D	-4.00	105.36	112.53
10	H	211	HEC	CMC-C2C-C1C	-3.94	121.85	128.36
10	B	211	HEC	CBA-CAA-C2A	-3.90	105.53	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	E	211	HEC	CBA-CAA-C2A	-3.89	105.55	112.53
10	C	322	HEC	CMC-C2C-C1C	-3.83	122.03	128.36
10	C	322	HEC	CAA-CBA-CGA	-3.83	105.73	112.75
5	A	502	HEM	CBA-CAA-C2A	-3.81	105.69	112.53
10	C	322	HEC	CBD-CAD-C3D	-3.78	105.76	112.53
5	A	502	HEM	C3B-CAB-CBB	-3.77	118.68	124.46
10	M	322	HEC	CBD-CAD-C3D	-3.73	105.85	112.53
10	F	322	HEC	CMC-C2C-C1C	-3.72	122.20	128.36
10	F	321	HEC	CMC-C2C-C1C	-3.67	122.29	128.36
10	L	211	HEC	CMC-C2C-C1C	-3.62	122.38	128.36
5	K	501	HEM	CAA-CBA-CGA	-3.55	106.23	112.75
5	G	502	HEM	CMA-C3A-C4A	-3.49	122.59	128.36
10	I	322	HEC	CMC-C2C-C1C	-3.39	122.75	128.36
5	A	501	HEM	CAA-CBA-CGA	-3.39	106.54	112.75
5	G	502	HEM	C3C-CAC-CBC	-3.31	119.37	124.46
5	A	501	HEM	C3C-CAC-CBC	-3.23	119.50	124.46
10	M	322	HEC	CMC-C2C-C1C	-3.22	123.04	128.36
10	I	322	HEC	CBD-CAD-C3D	-3.19	106.82	112.53
10	F	322	HEC	CBD-CAD-C3D	-3.15	106.89	112.53
5	A	502	HEM	C3C-CAC-CBC	-3.14	119.64	124.46
10	E	211	HEC	CMC-C2C-C1C	-3.12	123.19	128.36
5	D	501	HEM	CAA-CBA-CGA	-3.10	107.07	112.75
10	B	211	HEC	CMC-C2C-C1C	-3.08	123.27	128.36
10	M	322	HEC	CAD-CBD-CGD	-2.88	107.47	112.75
10	H	211	HEC	CAD-CBD-CGD	-2.86	107.50	112.75
10	I	321	HEC	CMB-C2B-C1B	-2.70	123.90	128.36
10	F	322	HEC	CAD-CBD-CGD	-2.69	107.82	112.75
5	D	502	HEM	C3B-CAB-CBB	-2.66	120.38	124.46
5	K	502	HEM	CMA-C3A-C4A	-2.65	123.99	128.36
10	I	322	HEC	CAA-CBA-CGA	-2.64	107.91	112.75
10	C	322	HEC	CBA-CAA-C2A	-2.63	107.81	112.53
10	C	322	HEC	CAD-CBD-CGD	-2.63	107.93	112.75
10	H	211	HEC	CAA-C2A-C1A	-2.62	124.16	127.01
5	G	501	HEM	CAA-C2A-C1A	-2.60	124.19	127.01
10	M	321	HEC	CMC-C2C-C1C	-2.59	124.08	128.36
10	M	321	HEC	CMB-C2B-C1B	-2.59	124.08	128.36
5	A	502	HEM	CMA-C3A-C4A	-2.58	124.10	128.36
10	F	322	HEC	CAA-CBA-CGA	-2.58	108.03	112.75
5	A	501	HEM	C3B-CAB-CBB	-2.53	120.57	124.46
5	D	502	HEM	CMA-C3A-C4A	-2.51	124.22	128.36
10	C	322	HEC	CAA-C2A-C1A	-2.39	124.41	127.01
10	I	322	HEC	CBA-CAA-C2A	-2.39	108.25	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	502	HEM	C3C-CAC-CBC	-2.36	120.84	124.46
10	C	321	HEC	CMB-C2B-C1B	-2.33	124.50	128.36
10	F	321	HEC	CMB-C2B-C1B	-2.32	124.53	128.36
10	F	322	HEC	CBA-CAA-C2A	-2.26	108.47	112.53
5	G	501	HEM	C3B-CAB-CBB	-2.22	121.05	124.46
10	L	211	HEC	CBD-CAD-C3D	-2.21	108.56	112.53
5	A	501	HEM	CAD-CBD-CGD	-2.16	104.20	113.02
5	K	502	HEM	C3B-CAB-CBB	-2.15	121.15	124.46
5	K	501	HEM	C3C-CAC-CBC	-2.13	121.19	124.46
5	G	502	HEM	C3B-CAB-CBB	-2.12	121.21	124.46
5	K	502	HEM	C3B-C4B-NB	-2.06	107.69	111.63
10	F	321	HEC	CAA-C2A-C1A	-2.01	124.83	127.01
5	G	501	HEM	C2C-C1C-CHC	2.03	126.77	123.68
5	K	501	HEM	C2C-C1C-CHC	2.05	126.79	123.68
5	K	501	HEM	C2D-C3D-C4D	2.07	105.01	101.50
5	G	501	HEM	C2D-C3D-C4D	2.09	105.04	101.50
5	D	501	HEM	C2D-C3D-C4D	2.12	105.09	101.50
10	M	321	HEC	CBA-CAA-C2A	2.14	116.36	112.53
5	D	501	HEM	C2C-C1C-CHC	2.14	126.93	123.68
5	A	501	HEM	C2D-C3D-C4D	2.15	105.15	101.50
5	D	501	HEM	C3B-C4B-CHC	2.16	126.21	123.16
10	M	322	HEC	CAD-C3D-C4D	2.22	129.41	127.01
5	A	502	HEM	CMC-C2C-C3C	2.26	122.17	116.53
5	G	501	HEM	C3B-C4B-CHC	2.27	126.36	123.16
5	K	501	HEM	C3B-C4B-CHC	2.39	126.53	123.16
5	D	502	HEM	C3B-C4B-CHC	2.52	126.71	123.16
10	H	211	HEC	CAD-C3D-C4D	2.54	129.76	127.01
5	A	502	HEM	CMD-C2D-C3D	2.58	125.78	114.35
10	I	322	HEC	CAD-C3D-C4D	2.61	129.84	127.01
5	K	502	HEM	CMC-C2C-C3C	2.65	123.15	116.53
5	G	501	HEM	CMD-C2D-C3D	2.66	126.12	114.35
10	L	211	HEC	CAD-C3D-C4D	2.69	129.93	127.01
5	G	502	HEM	C3B-C4B-CHC	2.78	127.08	123.16
5	K	502	HEM	CMD-C2D-C3D	2.79	126.71	114.35
5	D	502	HEM	CMC-C2C-C3C	2.83	123.60	116.53
5	K	501	HEM	CMD-C2D-C3D	2.92	127.27	114.35
5	D	502	HEM	CMD-C2D-C3D	2.96	127.42	114.35
5	A	501	HEM	C3B-C4B-CHC	2.98	127.36	123.16
5	A	501	HEM	CMD-C2D-C3D	3.01	127.65	114.35
5	G	502	HEM	CMD-C2D-C3D	3.05	127.82	114.35
5	D	501	HEM	CMD-C2D-C3D	3.09	128.01	114.35
5	G	502	HEM	CAA-CBA-CGA	3.10	118.42	112.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	502	HEM	C3B-C4B-CHC	3.13	127.57	123.16
5	G	502	HEM	CMC-C2C-C3C	3.13	124.35	116.53
5	D	502	HEM	CAA-CBA-CGA	3.17	118.56	112.75
10	C	322	HEC	CAD-C3D-C4D	3.39	130.69	127.01
5	K	502	HEM	C3B-C4B-CHC	3.45	128.03	123.16
5	A	502	HEM	CAA-CBA-CGA	3.50	119.17	112.75
5	A	501	HEM	CMC-C2C-C3C	3.67	125.69	116.53
5	G	502	HEM	CAD-C3D-C4D	3.76	125.74	112.47
5	D	501	HEM	CMC-C2C-C3C	3.91	126.28	116.53
5	G	501	HEM	CMB-C2B-C3B	3.97	126.43	116.53
5	K	501	HEM	CMC-C2C-C3C	3.99	126.48	116.53
5	A	501	HEM	CAD-C3D-C4D	3.99	126.53	112.47
5	D	501	HEM	CAD-C3D-C4D	4.02	126.66	112.47
5	K	502	HEM	CMB-C2B-C3B	4.11	126.79	116.53
5	K	501	HEM	CMB-C2B-C3B	4.12	126.81	116.53
5	K	501	HEM	CAD-C3D-C4D	4.12	127.01	112.47
5	G	501	HEM	CMC-C2C-C3C	4.18	126.97	116.53
10	B	211	HEC	CAD-C3D-C4D	4.22	131.59	127.01
5	D	501	HEM	CMB-C2B-C3B	4.23	127.08	116.53
5	K	502	HEM	CAD-C3D-C4D	4.26	127.50	112.47
5	D	502	HEM	CAD-C3D-C4D	4.31	127.67	112.47
5	G	501	HEM	CAD-C3D-C4D	4.37	127.89	112.47
5	A	502	HEM	CMB-C2B-C3B	4.38	127.47	116.53
5	A	502	HEM	CAD-C3D-C4D	4.39	127.97	112.47
5	D	502	HEM	CMB-C2B-C3B	4.44	127.61	116.53
5	G	502	HEM	CMB-C2B-C3B	4.75	128.38	116.53
5	G	501	HEM	CAD-C3D-C2D	4.81	127.04	113.22
5	A	501	HEM	CMB-C2B-C3B	4.94	128.86	116.53
5	A	502	HEM	CAD-C3D-C2D	5.06	127.77	113.22
5	D	502	HEM	CAD-C3D-C2D	5.07	127.80	113.22
5	K	501	HEM	CAD-C3D-C2D	5.12	127.93	113.22
5	D	501	HEM	CAD-C3D-C2D	5.21	128.21	113.22
5	A	501	HEM	CAD-C3D-C2D	5.24	128.29	113.22
5	K	502	HEM	CAD-C3D-C2D	5.25	128.30	113.22
5	G	502	HEM	CAD-C3D-C2D	5.74	129.72	113.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

24 monomers are involved in 124 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	501	HEM	5	0
5	A	502	HEM	6	0
10	B	211	HEC	3	0
10	C	321	HEC	7	0
10	C	322	HEC	3	0
11	C	323	FC6	4	0
5	D	501	HEM	4	0
5	D	502	HEM	8	0
10	E	211	HEC	2	0
10	F	321	HEC	11	0
10	F	322	HEC	6	0
11	F	323	FC6	10	0
5	G	501	HEM	6	0
5	G	502	HEM	7	0
10	H	211	HEC	4	0
10	I	321	HEC	4	0
10	I	322	HEC	2	0
11	I	323	FC6	6	0
5	K	501	HEM	5	0
5	K	502	HEM	7	0
10	L	211	HEC	2	0
10	M	321	HEC	5	0
10	M	322	HEC	4	0
11	M	323	FC6	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	466/474 (98%)	-0.75	5 (1%) 82 72	44, 75, 127, 177	0
1	D	463/474 (97%)	-0.28	20 (4%) 39 25	73, 156, 249, 313	0
1	G	465/474 (98%)	-0.68	3 (0%) 90 84	54, 88, 133, 176	0
1	K	465/474 (98%)	-0.37	14 (3%) 54 39	64, 145, 232, 269	0
2	B	197/203 (97%)	-0.79	1 (0%) 91 87	39, 64, 124, 172	0
2	E	197/203 (97%)	-0.18	9 (4%) 36 23	66, 140, 243, 290	0
2	H	197/203 (97%)	-0.68	4 (2%) 68 54	50, 78, 144, 200	0
2	L	197/203 (97%)	-0.52	6 (3%) 54 39	51, 105, 244, 304	0
3	C	303/311 (97%)	-0.64	3 (0%) 84 75	41, 77, 123, 179	0
3	F	303/311 (97%)	0.19	16 (5%) 30 17	71, 182, 279, 333	0
3	I	303/311 (97%)	-0.45	6 (1%) 68 54	48, 100, 158, 209	0
3	M	303/311 (97%)	-0.38	10 (3%) 50 35	43, 81, 279, 345	0
4	U	0/30	-	-	-	-
4	X	0/30	-	-	-	-
4	Y	0/30	-	-	-	-
4	Z	0/30	-	-	-	-
All	All	3859/4072 (94%)	-0.46	97 (2%) 61 47	39, 103, 235, 345	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	201	ASN	11.8
3	F	3	THR	9.0
2	E	202	LYS	8.2
1	K	299	HIS	7.3
3	F	34	GLY	5.8
2	E	37	ASP	5.6
3	M	34	GLY	5.2

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Mol	Chain	Res	Type	RSRZ
1	D	467	TYR	5.1
1	D	299	HIS	5.1
3	F	163	GLN	5.0
1	G	8	ALA	4.7
3	F	33	ALA	4.5
3	M	35	THR	4.4
1	D	153	LYS	4.3
1	D	296	GLY	4.3
3	M	43	ALA	4.2
3	I	42	HIS	4.2
2	E	44	GLU	4.2
2	H	202	LYS	4.1
1	D	302	ARG	4.1
1	A	5	THR	4.1
1	D	374	GLN	4.1
3	F	2	SER	4.0
1	K	153	LYS	4.0
1	D	464	PRO	4.0
1	D	8	ALA	3.9
3	I	35	THR	3.6
1	D	470	ALA	3.5
2	E	7	LEU	3.5
1	K	150	ALA	3.3
1	D	373	GLU	3.2
2	E	9	LYS	3.2
1	D	456	TRP	3.1
2	E	13	LEU	3.1
1	K	156	HIS	3.1
3	M	42	HIS	3.1
1	K	302	ARG	3.1
1	D	86	GLN	3.1
3	F	4	PHE	3.0
1	D	466	GLU	3.0
2	H	7	LEU	3.0
3	M	51	ASP	2.9
1	D	93	LYS	2.9
3	F	35	THR	2.8
3	I	3	THR	2.8
1	G	7	THR	2.8
3	M	37	ASP	2.8
2	E	170	GLU	2.8
1	K	7	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	465	ALA	2.8
3	F	30	GLY	2.7
2	L	9	LYS	2.6
1	A	6	SER	2.6
3	M	88	GLY	2.6
3	F	53	PRO	2.6
3	F	283	GLN	2.6
3	F	239	GLN	2.6
1	K	465	ALA	2.5
3	I	90	GLU	2.5
3	F	42	HIS	2.5
3	M	38	GLN	2.5
1	A	373	GLU	2.5
2	B	202	LYS	2.5
1	A	155	LYS	2.5
1	A	7	THR	2.5
2	L	202	LYS	2.4
1	K	6	SER	2.4
2	L	11	VAL	2.4
2	E	35	PHE	2.4
3	C	29	LYS	2.4
1	K	96	ALA	2.4
1	D	231	GLU	2.4
1	D	463	LYS	2.4
3	M	82	TRP	2.4
2	L	35	PHE	2.3
1	K	466	GLU	2.3
1	K	374	GLN	2.2
1	G	6	SER	2.2
3	M	53	PRO	2.2
3	C	30	GLY	2.2
2	H	10	ASN	2.2
3	F	87	PRO	2.2
3	C	108	GLU	2.2
1	K	8	ALA	2.2
2	L	10	ASN	2.2
1	K	468	ASP	2.1
3	F	22	TRP	2.1
1	D	384	HIS	2.1
1	K	231	GLU	2.1
3	I	30	GLY	2.1
3	F	130	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
2	H	9	LYS	2.1
3	I	88	GLY	2.0
3	F	149	SER	2.0
1	D	298	TRP	2.0
1	D	192	LEU	2.0
2	L	151	LYS	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
11	FC6	I	323	13/13	0.89	0.36	4.78	52,57,68,80	13
11	FC6	F	323	13/13	0.86	0.31	3.51	37,40,42,46	13
9	PO4	G	506	5/5	0.94	0.27	2.52	27,29,32,35	0
11	FC6	C	323	13/13	0.96	0.25	1.60	33,39,46,55	13
5	HEM	K	501	43/43	0.95	0.22	1.22	117,127,147,153	0
10	HEC	F	322	43/43	0.94	0.25	1.08	34,43,47,50	0
9	PO4	A	506	5/5	0.95	0.19	0.99	21,22,23,24	0
8	PEO	K	508	2/2	0.99	0.17	0.65	130,130,130,135	0
10	HEC	F	321	43/43	0.94	0.23	0.65	20,24,28,35	0
11	FC6	M	323	13/13	0.97	0.17	0.42	28,30,38,39	13
10	HEC	E	211	43/43	0.97	0.15	0.32	16,18,27,32	0
5	HEM	K	502	43/43	0.97	0.16	0.23	85,102,115,125	0
5	HEM	D	502	43/43	0.98	0.15	0.18	83,96,110,112	0
5	HEM	A	502	43/43	0.98	0.14	0.10	43,52,61,72	0
10	HEC	L	211	43/43	0.97	0.12	-0.16	18,21,26,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	HEM	D	501	43/43	0.98	0.14	-0.26	96,121,137,149	0
5	HEM	G	502	43/43	0.98	0.12	-0.38	56,61,70,83	0
10	HEC	I	322	43/43	0.98	0.10	-0.47	24,28,31,36	0
10	HEC	B	211	43/43	0.98	0.10	-0.59	25,28,35,46	0
5	HEM	G	501	43/43	0.99	0.11	-0.65	56,71,81,89	0
10	HEC	I	321	43/43	0.98	0.10	-0.67	20,24,34,39	0
7	CA	G	505	1/1	0.93	0.12	-0.67	91,91,91,91	0
5	HEM	A	501	43/43	0.99	0.11	-0.68	47,57,64,71	0
10	HEC	H	211	43/43	0.98	0.10	-0.74	24,27,32,38	0
9	PO4	D	506	5/5	0.81	0.19	-0.83	177,178,188,191	0
10	HEC	C	321	43/43	0.99	0.08	-0.87	21,27,36,44	0
10	HEC	C	322	43/43	0.98	0.10	-0.91	22,28,34,36	0
10	HEC	M	322	43/43	0.98	0.09	-0.94	19,23,27,34	0
7	CA	A	505	1/1	0.71	0.11	-1.01	88,88,88,88	0
10	HEC	M	321	43/43	0.99	0.09	-1.10	18,25,35,43	0
8	PEO	D	508	2/2	0.99	0.12	-1.33	133,133,133,141	0
8	PEO	G	508	2/2	1.00	0.10	-1.52	71,71,71,74	0
7	CA	K	505	1/1	0.95	0.08	-1.58	133,133,133,133	0
7	CA	D	505	1/1	0.80	0.10	-1.62	138,138,138,138	0
7	CA	E	504	1/1	0.99	0.09	-1.63	105,105,105,105	0
9	PO4	K	506	5/5	0.95	0.08	-1.78	140,144,146,153	0
8	PEO	A	508	2/2	1.00	0.10	-1.84	57,57,57,63	0
7	CA	K	504	1/1	0.97	0.05	-2.82	99,99,99,99	0
7	CA	B	504	1/1	1.00	0.11	-	51,51,51,51	0
7	CA	G	504	1/1	0.98	0.08	-	74,74,74,74	0
6	CU	K	503	1/1	0.98	0.11	-	135,135,135,135	0
6	CU	G	503	1/1	0.99	0.05	-	77,77,77,77	0
6	CU	D	503	1/1	0.98	0.05	-	115,115,115,115	0
6	CU	A	503	1/1	1.00	0.09	-	59,59,59,59	0

6.5 Other polymers ⓘ

There are no such residues in this entry.