



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 25, 2017 – 06:53 PM EDT

PDB ID : 3L71
Title : Cytochrome BC1 complex from chicken with azoxystrobin bound
Authors : Huang, L.; Berry, E.A.
Deposited on : unknown
Resolution : 2.84 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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-20030345

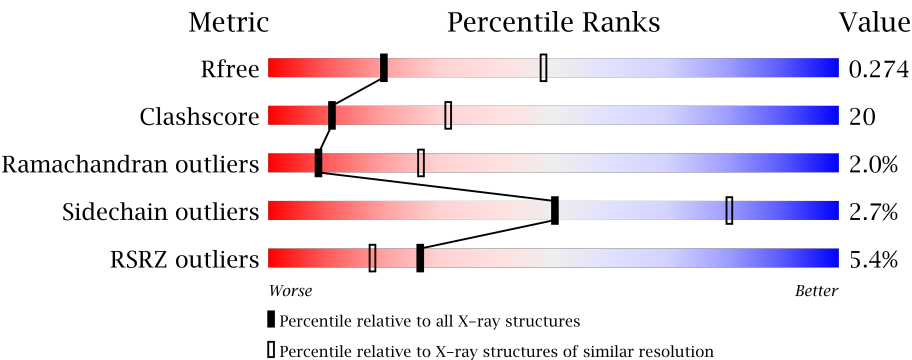
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.84 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}	100719	3466 (2.88-2.80)
Clashscore	112137	3975 (2.88-2.80)
Ramachandran outliers	110173	3902 (2.88-2.80)
Sidechain outliers	110143	3905 (2.88-2.80)
RSRZ outliers	101464	3501 (2.88-2.80)

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	446	<div><div>3%</div><div>65%</div><div>32%</div><div>.</div></div>
1	N	446	<div><div>3%</div><div>60%</div><div>36%</div><div>..</div></div>
2	B	441	<div><div>5%</div><div>51%</div><div>40%</div><div>. 5%</div></div>
2	O	441	<div><div>4%</div><div>54%</div><div>37%</div><div>. .</div></div>
3	C	380	<div><div>2%</div><div>78%</div><div>21%</div><div>.</div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	P	380	
4	D	241	
4	Q	241	
5	E	196	
5	R	196	
6	F	110	
6	S	110	
7	G	81	
7	T	81	
8	H	77	
8	U	77	
9	I	47	
9	V	47	
10	J	61	
10	W	61	

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	PEE	A	2005	-	-	-	X
11	PEE	A	2008	-	-	-	X
11	PEE	C	2007	-	-	-	X
11	PEE	N	3008	-	X	-	-
11	PEE	P	3005	-	-	-	X
11	PEE	P	3007	-	-	-	X
14	UQ	C	2002	-	-	-	X
14	UQ	P	3002	-	-	-	X
15	GOL	P	3011	-	-	-	X
19	FES	E	501	-	-	X	-
19	FES	R	501	-	-	X	-

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 32655 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 Mitochondrial ubiquinol-cytochrome-c reductase complex core protein i.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	444	Total	C	N	O	S	0	0	0
			3447	2160	607	659	21			
1	N	442	Total	C	N	O	S	0	0	0
			3437	2154	605	657	21			

- Molecule 2 is a protein called Mitochondrial ubiquinol-cytochrome-c reductase complex core protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	420	Total	C	N	O	S	0	0	0
			3133	1968	544	612	9			
2	O	422	Total	C	N	O	S	0	0	0
			3147	1977	546	614	10			

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	380	Total	C	N	O	S	0	0	0
			3017	2022	478	505	12			
3	P	379	Total	C	N	O	S	0	0	0
			3012	2019	477	504	12			

- Molecule 4 is a protein called Mitochondrial cytochrome c1, heme protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	241	Total	C	N	O	S	0	0	0
			1898	1212	327	347	12			
4	Q	241	Total	C	N	O	S	0	0	0
			1898	1212	327	347	12			

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	196	Total	C	N	O	S	0	0	0
			1513	952	263	292	6			
5	R	196	Total	C	N	O	S	0	0	0
			1509	950	263	290	6			

- Molecule 6 is a protein called Mitochondrial ubiquinol-cytochrome c reductase 14 kda protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	101	Total	C	N	O	S	0	0	0
			891	570	159	159	3			
6	S	101	Total	C	N	O	S	0	0	0
			891	570	159	159	3			

- Molecule 7 is a protein called Mitochondrial ubiquinol-cytochrome c reductase ubiquinone-binding protein qp-c.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	80	Total	C	N	O		0	0	0
			672	437	119	116				
7	T	79	Total	C	N	O		0	0	0
			662	432	117	113				

- Molecule 8 is a protein called Mitochondrial ubiquinol-cytochrome c reductase 11 kda protein, complex iii subunit viii.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	70	Total	C	N	O	S	0	0	0
			574	350	105	114	5			
8	U	67	Total	C	N	O	S	0	0	0
			553	338	103	107	5			

- Molecule 9 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	46	Total	C	N	O	S	0	0	0
			287	171	58	56	2			
9	V	43	Total	C	N	O	S	0	0	0
			277	167	55	53	2			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	28	UNK	-	INSERTION	UNP Q5ZLR5

Continued on next page...

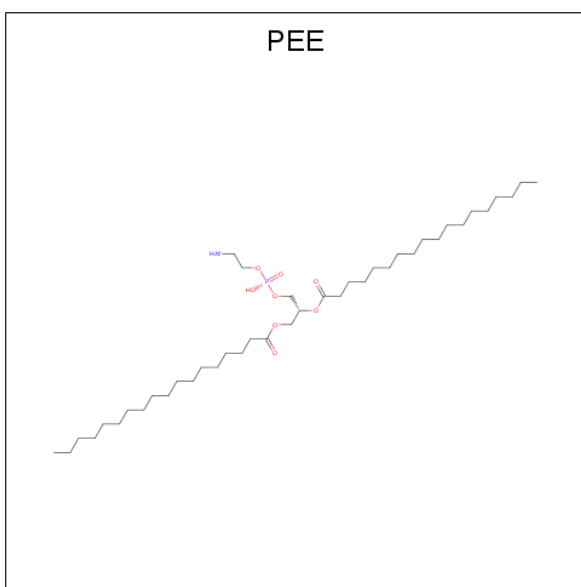
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
I	29	UNK	-	INSERTION	UNP Q5ZLR5
I	30	UNK	-	INSERTION	UNP Q5ZLR5
I	31	UNK	-	INSERTION	UNP Q5ZLR5
I	32	UNK	-	INSERTION	UNP Q5ZLR5
I	33	UNK	-	INSERTION	UNP Q5ZLR5
I	34	UNK	-	INSERTION	UNP Q5ZLR5
I	35	UNK	-	INSERTION	UNP Q5ZLR5
I	36	UNK	-	INSERTION	UNP Q5ZLR5
I	37	UNK	-	INSERTION	UNP Q5ZLR5
I	38	UNK	-	INSERTION	UNP Q5ZLR5
I	39	UNK	-	INSERTION	UNP Q5ZLR5
I	40	UNK	-	INSERTION	UNP Q5ZLR5
I	41	UNK	-	INSERTION	UNP Q5ZLR5
I	42	UNK	-	INSERTION	UNP Q5ZLR5
V	25	UNK	-	INSERTION	UNP Q5ZLR5
V	26	UNK	-	INSERTION	UNP Q5ZLR5
V	27	UNK	-	INSERTION	UNP Q5ZLR5
V	28	UNK	-	INSERTION	UNP Q5ZLR5
V	29	UNK	-	INSERTION	UNP Q5ZLR5
V	30	UNK	-	INSERTION	UNP Q5ZLR5
V	31	UNK	-	INSERTION	UNP Q5ZLR5
V	32	UNK	-	INSERTION	UNP Q5ZLR5
V	33	UNK	-	INSERTION	UNP Q5ZLR5
V	35	UNK	-	INSERTION	UNP Q5ZLR5
V	36	UNK	-	INSERTION	UNP Q5ZLR5
V	37	UNK	-	INSERTION	UNP Q5ZLR5
V	38	UNK	-	INSERTION	UNP Q5ZLR5
V	39	UNK	-	INSERTION	UNP Q5ZLR5
V	40	UNK	-	INSERTION	UNP Q5ZLR5

- Molecule 10 is a protein called Mitochondrial ubiquinol-cytochrome c reductase 7.2 kda protein.

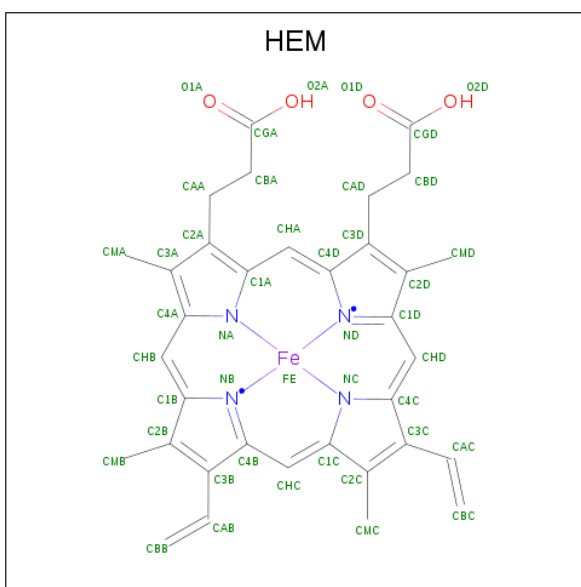
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	61	Total	C	N	O	0	0	0
			497	321	87	89			
10	W	60	Total	C	N	O	0	0	1
			479	311	86	82			

- Molecule 11 is 1,2-Dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula: C₄₁H₈₃NO₈P).



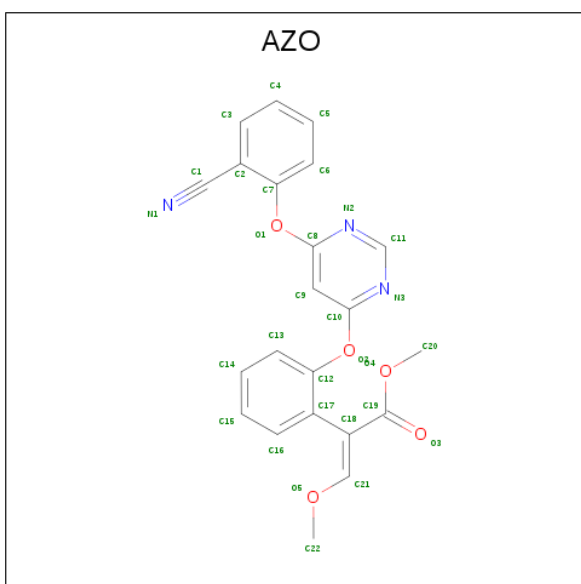
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	A	1	Total	C	N	O	P	0	0
			50	40	1	8	1		
11	A	1	Total	C	O	P		0	0
			21	12	8	1			
11	C	1	Total	C	N	O	P	0	0
			49	39	1	8	1		
11	N	1	Total	O	P			0	0
			5	4	1				
11	P	1	Total	C	N	O	P	0	0
			50	40	1	8	1		
11	P	1	Total	C	N	O	P	0	0
			49	39	1	8	1		

- Molecule 12 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



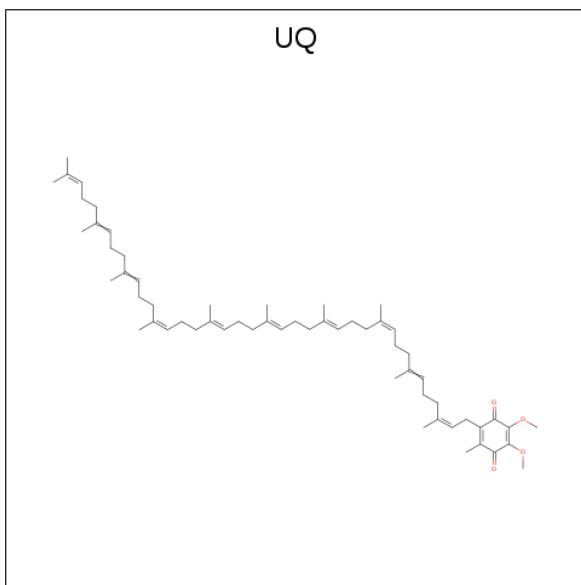
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
12	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
12	P	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
12	P	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 13 is METHYL (2Z)-2-(2-{[6-(2-CYANOPHENOXY)PYRIMIDIN-4-YL]OXY}PHENYL)-3-METHOXYACRYLATE (three-letter code: AZO) (formula: C₂₂H₁₇N₃O₅).



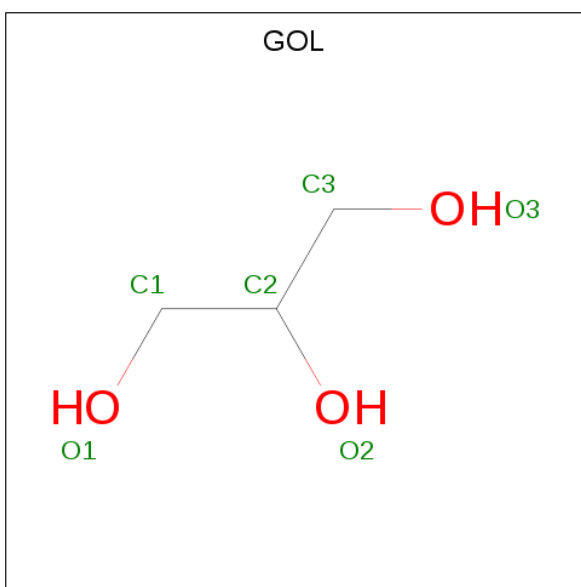
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	C	1	Total	C	N	O	0	0
			30	22	3	5		
13	P	1	Total	C	N	O	0	0
			30	22	3	5		

- Molecule 14 is Coenzyme Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-isomer (three-letter code: UQ) (formula: C₅₉H₉₀O₄).



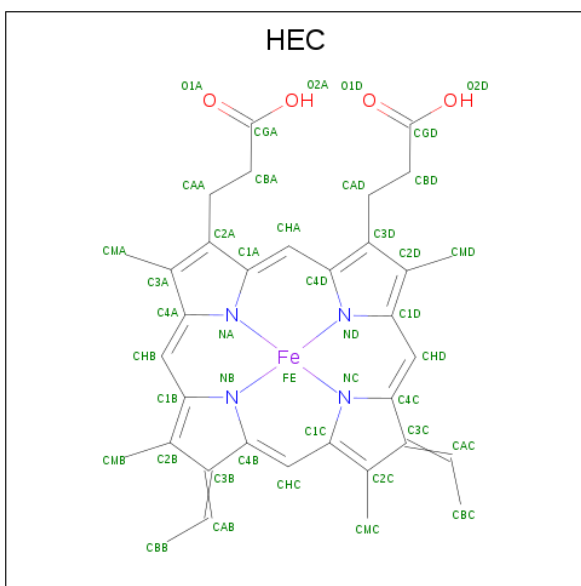
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	C	1	Total	C	O	0	0
			19	15	4		
14	P	1	Total	C	O	0	0
			19	15	4		

- Molecule 15 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



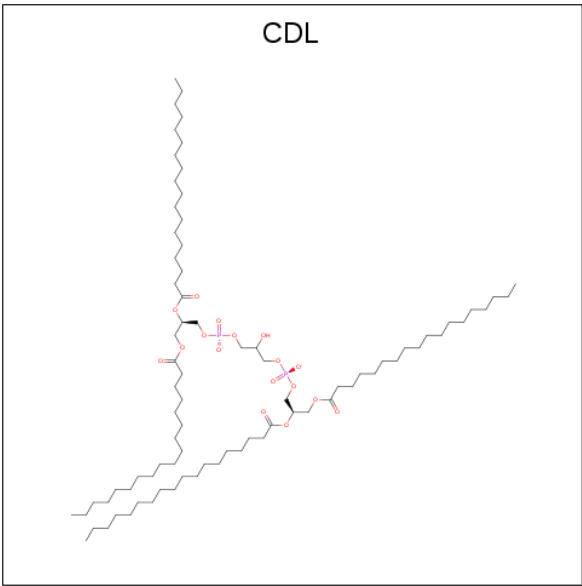
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	C	1	Total 6	C 3	O 3	0	0
15	P	1	Total 6	C 3	O 3	0	0

- Molecule 16 is HEME C (three-letter code: HEC) (formula: $\text{C}_{34}\text{H}_{34}\text{FeN}_4\text{O}_4$).



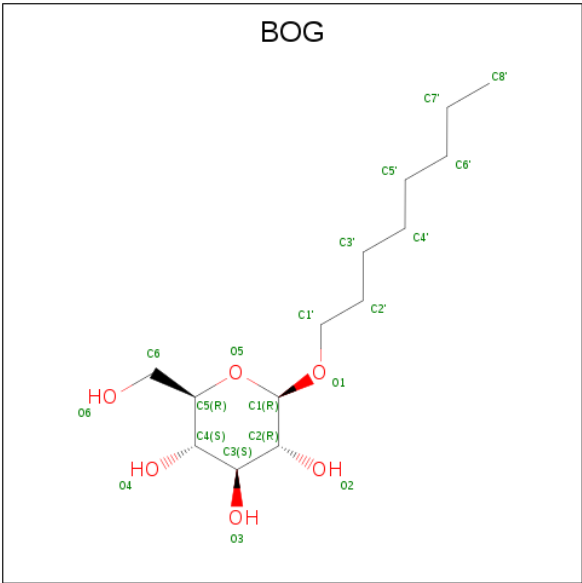
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
16	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
16	Q	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 17 is CARDIOLIPIN (three-letter code: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



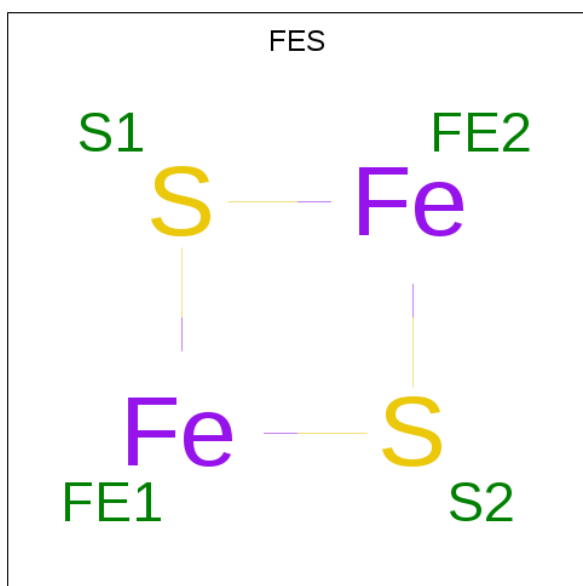
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	D	1	Total	C	O	P	0	0
			42	23	17	2		
17	G	1	Total	C	O	P	0	0
			40	21	17	2		
17	Q	1	Total	C	O	P	0	0
			42	23	17	2		
17	T	1	Total	C	O	P	0	0
			40	21	17	2		

- Molecule 18 is B-OCTYLGLUCOSIDE (three-letter code: BOG) (formula: C₁₄H₂₈O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	D	1	Total	C	O	0	0
			20	14	6		
18	D	1	Total	C	O	0	0
			13	7	6		
18	P	1	Total	C	O	0	0
			12	6	6		
18	Q	1	Total	C	O	0	0
			20	14	6		
18	Q	1	Total	C	O	0	0
			13	7	6		

- Molecule 19 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	E	1	Total	Fe	S	0	0
			4	2	2		
19	R	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 20 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	C	8	Total	O	0	0
			8	8		
20	E	1	Total	O	0	0
			1	1		
20	P	9	Total	O	0	0
			9	9		

Continued on next page...

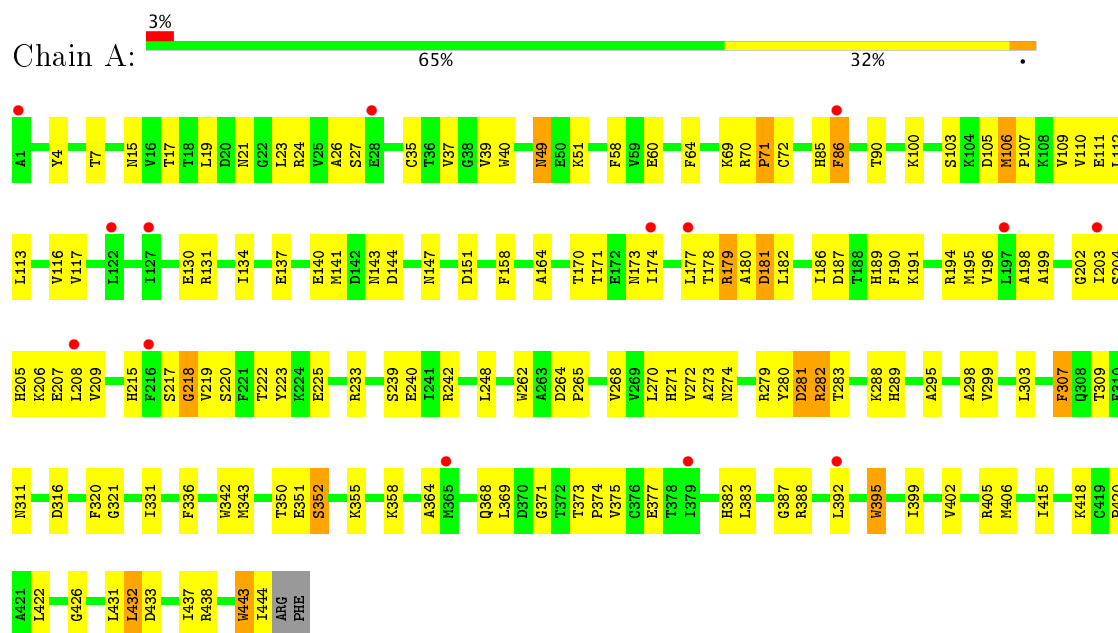
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	R	1	Total	O	0	0
			1	1		

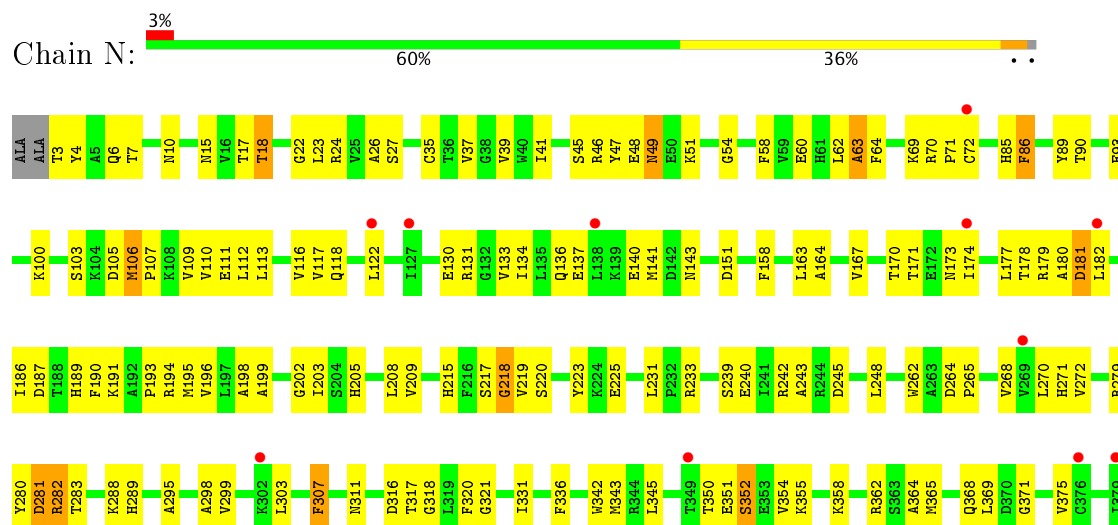
3 Residue-property plots

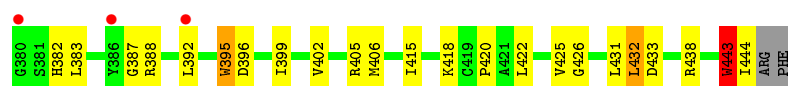
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

- Molecule 1: Mitochondrial ubiquinol-cytochrome-c reductase complex core protein i

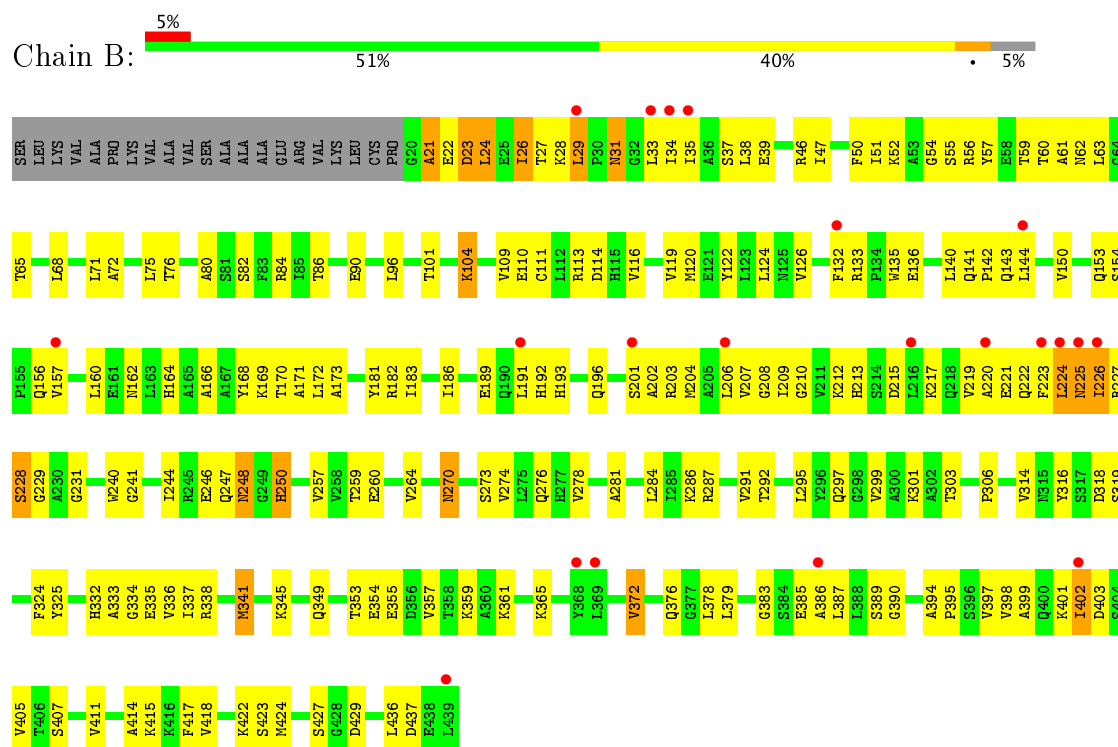


- Molecule 1: Mitochondrial ubiquinol-cytochrome-c reductase complex core protein i

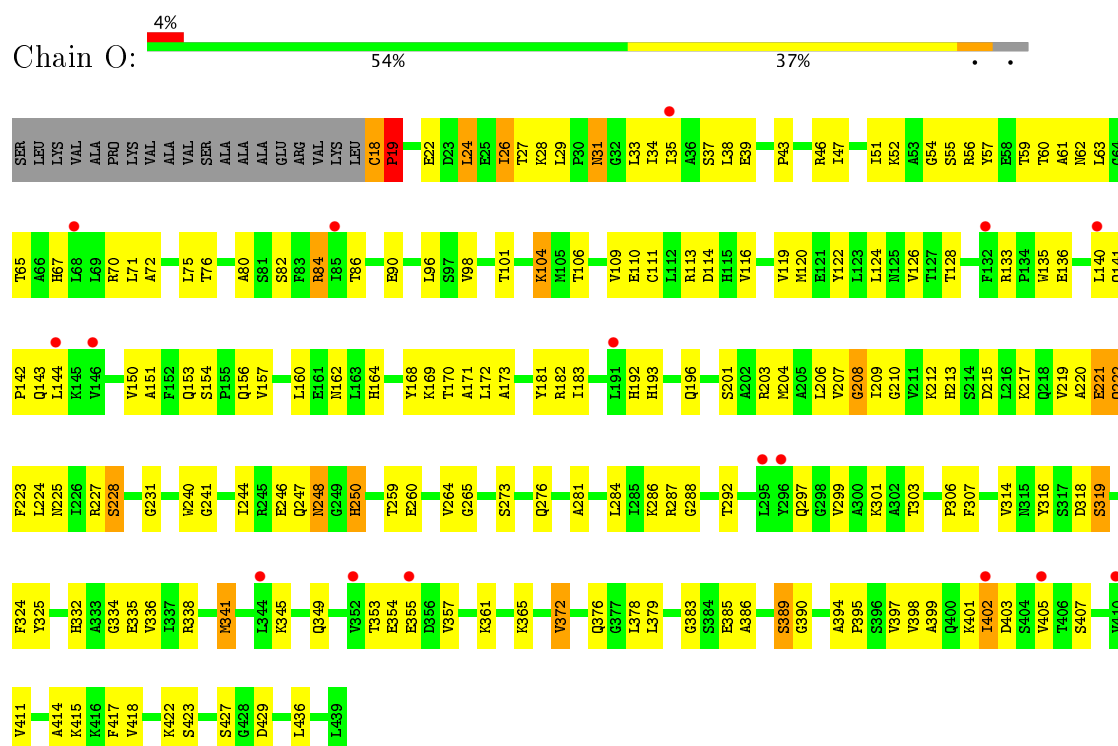




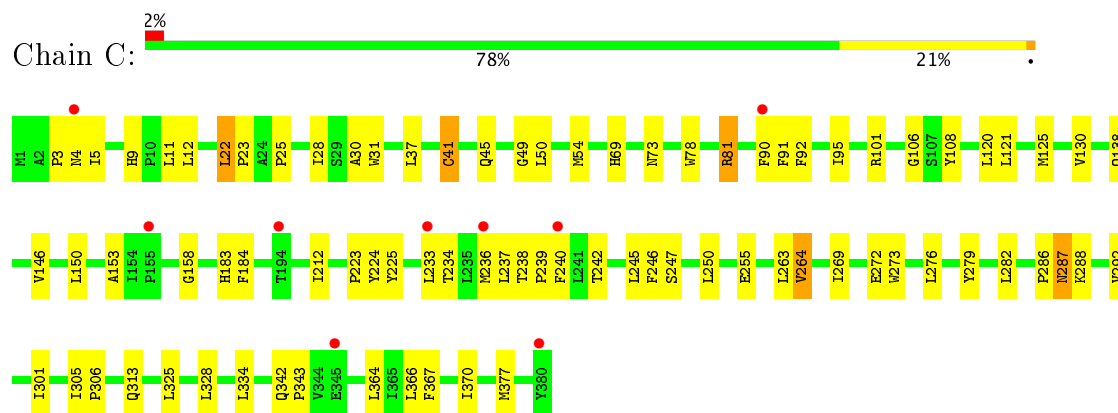
• Molecule 2: Mitochondrial ubiquinol-cytochrome-c reductase complex core protein 2



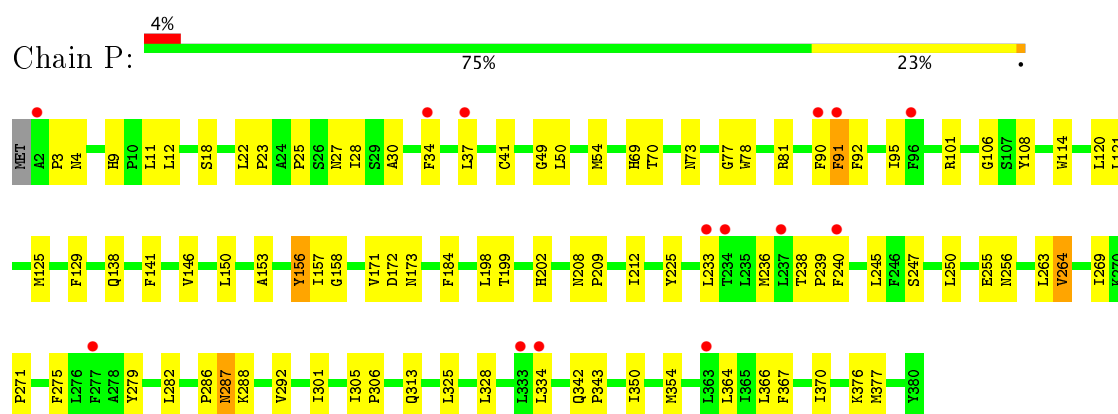
• Molecule 2: Mitochondrial ubiquinol-cytochrome-c reductase complex core protein 2



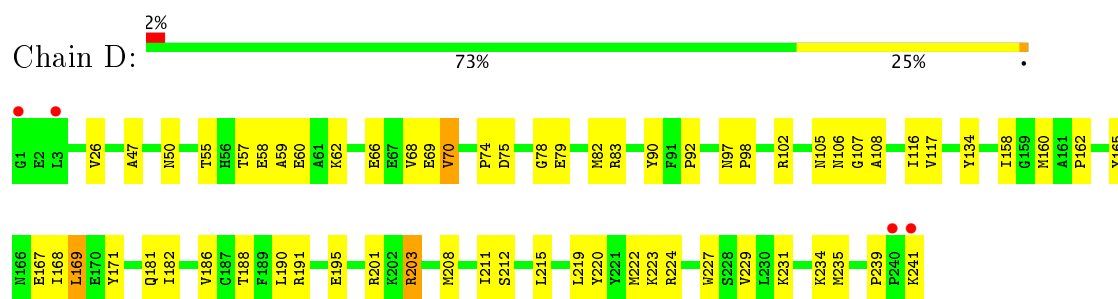
- Molecule 3: Cytochrome b



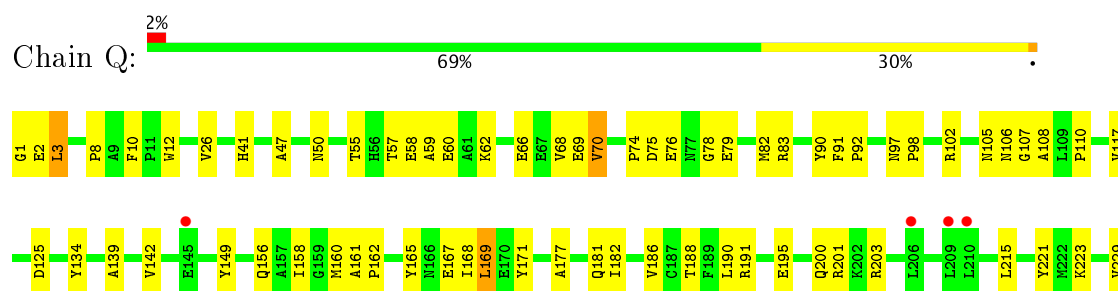
- Molecule 3: Cytochrome b



- Molecule 4: Mitochondrial cytochrome c1, heme protein

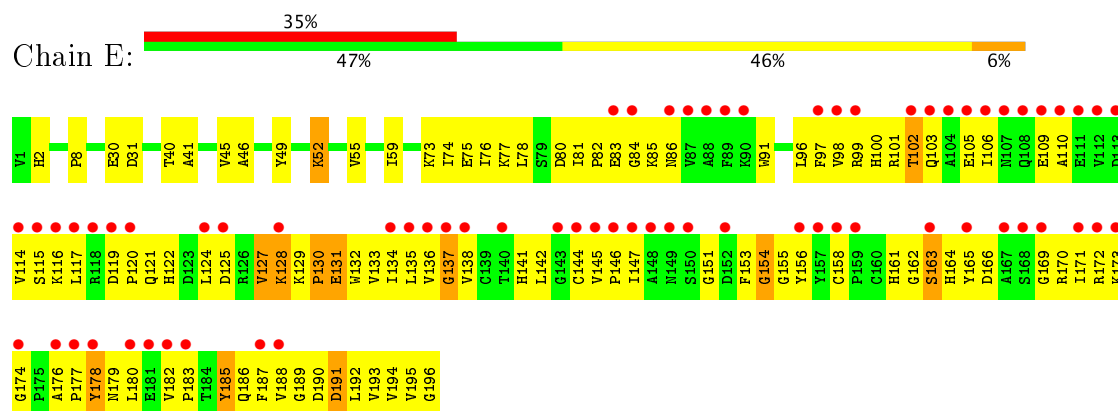


- Molecule 4: Mitochondrial cytochrome c1, heme protein

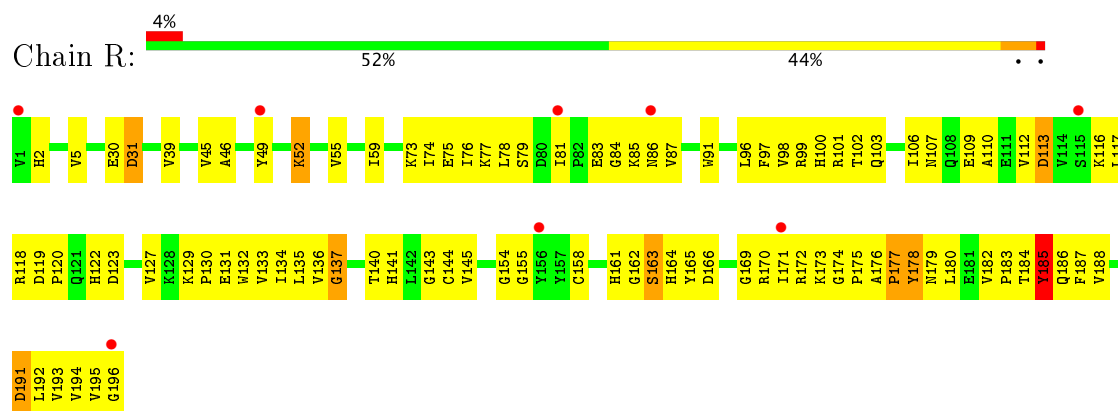




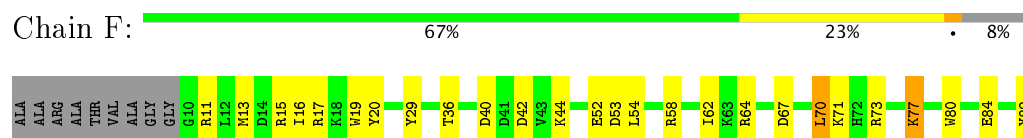
- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial



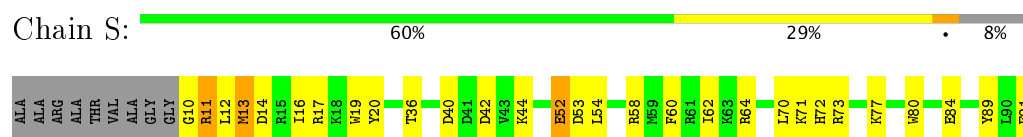
- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial



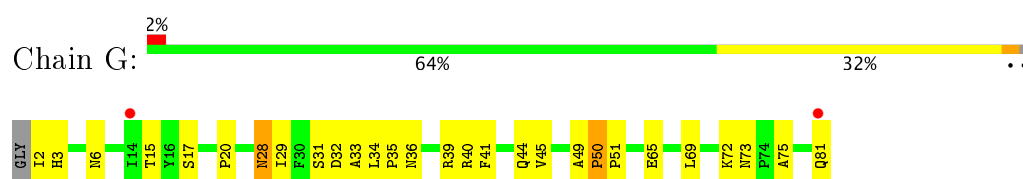
- Molecule 6: Mitochondrial ubiquinol-cytochrome c reductase 14 kda protein



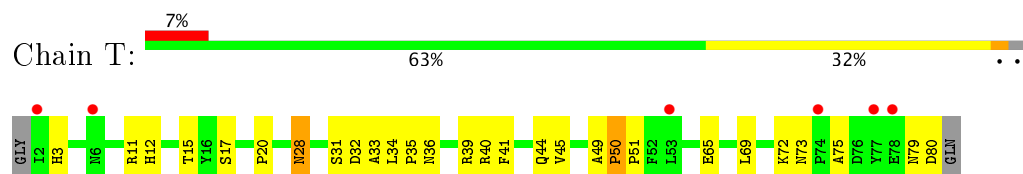
- Molecule 6: Mitochondrial ubiquinol-cytochrome c reductase 14 kda protein



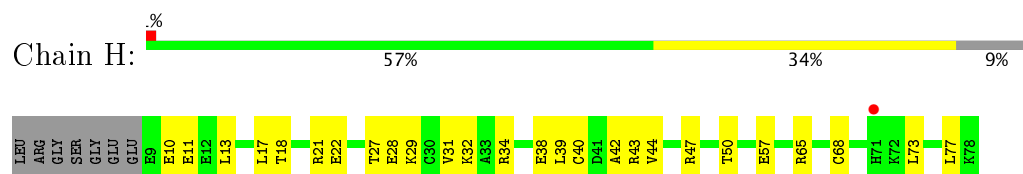
- Molecule 7: Mitochondrial ubiquinol-cytochrome c reductase ubiquinone-binding protein qp-c



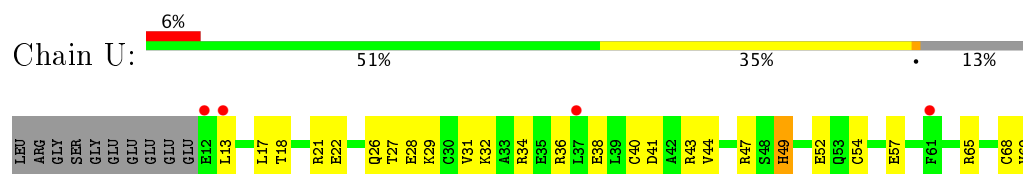
- Molecule 7: Mitochondrial ubiquinol-cytochrome c reductase ubiquinone-binding protein qp-c



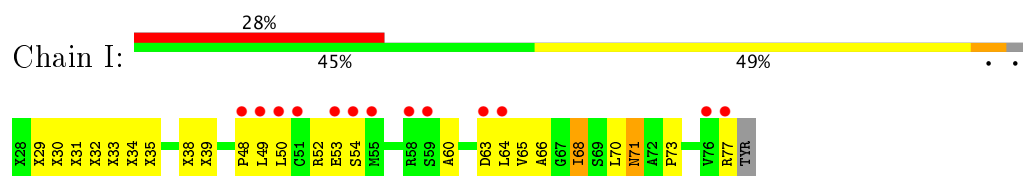
- Molecule 8: Mitochondrial ubiquinol-cytochrome c reductase 11 kda protein, complex iii subunit viii



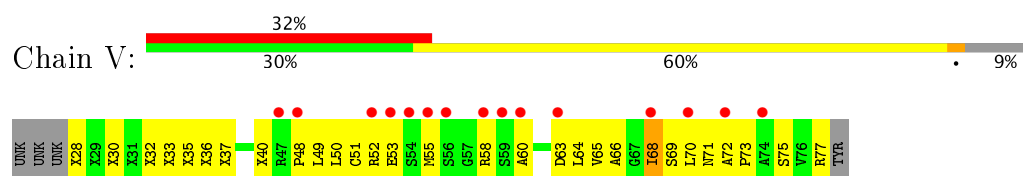
- Molecule 8: Mitochondrial ubiquinol-cytochrome c reductase 11 kda protein, complex iii subunit viii



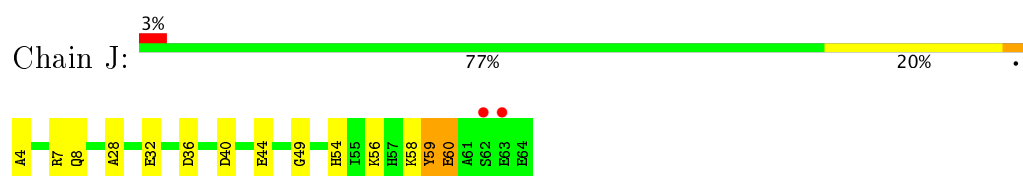
- Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial



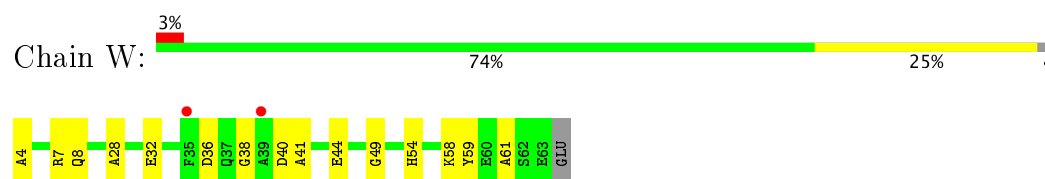
- Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial



- Molecule 10: Mitochondrial ubiquinol-cytochrome c reductase 7.2 kda protein



- Molecule 10: Mitochondrial ubiquinol-cytochrome c reductase 7.2 kda protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	170.15Å 181.31Å 240.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.94 – 2.84 144.78 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.5 (24.94-2.84) 93.6 (144.78-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 2.82Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.247 , 0.281 0.239 , 0.274	Depositor DCC
R_{free} test set	3237 reflections (2.00%)	DCC
Wilson B-factor (Å ²)	68.8	Xtriage
Anisotropy	0.675	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 55.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	32655	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.05% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, AZO, CDL, UQ, FES, HEC, PEE, HEM, BOG

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	0.44	0/3518	0.66	0/4767
1	N	0.42	0/3508	0.65	0/4753
2	B	0.39	0/3187	0.62	0/4321
2	O	0.40	0/3202	0.63	0/4343
3	C	0.51	0/3119	0.67	0/4270
3	P	0.46	0/3114	0.65	0/4263
4	D	0.47	0/1956	0.63	0/2658
4	Q	0.38	0/1956	0.61	0/2658
5	E	0.37	0/1547	0.59	0/2103
5	R	0.37	0/1543	0.60	1/2098 (0.0%)
6	F	0.53	0/911	0.65	0/1219
6	S	0.44	0/911	0.60	0/1219
7	G	0.49	0/694	0.66	0/941
7	T	0.42	0/684	0.62	0/929
8	H	0.42	0/582	0.63	0/779
8	U	0.32	0/561	0.57	0/751
9	I	0.39	0/218	0.58	0/293
9	V	0.37	0/218	0.59	0/293
10	J	0.43	0/508	0.60	0/682
10	W	0.40	0/490	0.60	0/660
All	All	0.43	0/32427	0.63	1/44000 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	R	143	GLY	N-CA-C	5.62	127.15	113.10

There are no chirality outliers.

There are no planarity outliers.

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	3447	0	3362	125	0
1	N	3437	0	3349	148	0
2	B	3133	0	3130	192	0
2	O	3147	0	3146	189	0
3	C	3017	0	3063	69	0
3	P	3012	0	3058	85	0
4	D	1898	0	1846	54	0
4	Q	1898	0	1846	66	0
5	E	1513	0	1478	114	0
5	R	1509	0	1474	101	0
6	F	891	0	893	20	0
6	S	891	0	893	31	0
7	G	672	0	653	30	0
7	T	662	0	645	34	0
8	H	574	0	548	20	0
8	U	553	0	535	27	0
9	I	287	0	250	38	0
9	V	277	0	249	38	0
10	J	497	0	490	16	0
10	W	479	0	478	16	0
11	A	71	0	90	0	0
11	C	49	0	72	5	0
11	N	5	0	0	0	0
11	P	99	0	149	3	0
12	C	86	0	60	5	0
12	P	86	0	60	4	0
13	C	30	0	17	0	0
13	P	30	0	17	2	0
14	C	19	0	17	4	0
14	P	19	0	17	6	0
15	C	6	0	8	1	0
15	P	6	0	8	0	0
16	D	43	0	30	3	0
16	Q	43	0	30	2	0
17	D	42	0	28	4	0
17	G	40	0	24	4	0
17	Q	42	0	28	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	T	40	0	24	3	0
18	D	33	0	39	1	0
18	P	12	0	11	1	0
18	Q	33	0	39	1	0
19	E	4	0	0	2	0
19	R	4	0	0	2	0
20	C	8	0	0	0	0
20	E	1	0	0	0	0
20	P	9	0	0	1	0
20	R	1	0	0	0	0
All	All	32655	0	32154	1295	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 (1295) 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)
5:E:121:GLN:HG2	5:E:170:ARG:HD3	1.14	1.11
9:I:33:UNK:HG2	9:I:73:PRO:HB3	1.12	1.09
2:O:353:THR:HG22	2:O:355:GLU:H	1.14	1.07
2:O:76:THR:HG22	2:O:82:SER:H	1.16	1.07
2:B:353:THR:HG22	2:B:355:GLU:H	1.17	1.07
2:O:51:ILE:HG12	2:O:204:MET:HG2	1.37	1.04
2:B:76:THR:HG22	2:B:82:SER:H	1.17	1.03
2:O:338:ARG:HH11	2:O:338:ARG:HG3	1.24	0.99
1:A:178:THR:HG22	1:A:180:ALA:H	1.24	0.98
1:N:178:THR:HG22	1:N:180:ALA:H	1.24	0.97
2:B:338:ARG:HG3	2:B:338:ARG:HH11	1.26	0.97
4:Q:47:ALA:H	4:Q:50:ASN:HD22	1.07	0.96
2:O:157:VAL:HG23	9:V:64:LEU:HD21	1.45	0.96
5:E:136:VAL:HG23	5:E:183:PRO:HD3	1.49	0.95
3:C:328:LEU:HD12	7:G:51:PRO:HB3	1.47	0.95
2:O:37:SER:HB3	2:O:213:HIS:ND1	1.81	0.94
2:O:314:VAL:HG13	9:V:63:ASP:HB3	1.49	0.94
4:D:57:THR:HG22	4:D:59:ALA:H	1.32	0.93
2:B:124:LEU:HD11	2:B:223:PHE:HB3	1.51	0.92
4:D:47:ALA:H	4:D:50:ASN:HD22	1.05	0.92
3:P:328:LEU:HD12	7:T:51:PRO:HB3	1.50	0.92
2:B:341:MET:HE1	2:B:417:PHE:HE2	1.31	0.92
2:B:157:VAL:HG23	9:I:64:LEU:HD21	1.51	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:27:THR:HG22	2:O:28:LYS:H	1.33	0.90
9:I:33:UNK:HG2	9:I:73:PRO:CB	2.00	0.89
1:N:106:MET:HG3	1:N:203:ILE:HD13	1.57	0.87
7:T:41:PHE:O	7:T:45:VAL:HG23	1.74	0.87
2:O:341:MET:HE1	2:O:417:PHE:HE2	1.40	0.86
4:Q:57:THR:HG22	4:Q:59:ALA:H	1.39	0.86
1:N:10:ASN:ND2	2:O:19:PRO:HD2	1.91	0.86
9:V:64:LEU:HD12	9:V:77:ARG:O	1.75	0.86
9:I:32:UNK:N	9:I:73:PRO:HG2	1.90	0.85
7:G:41:PHE:O	7:G:45:VAL:HG23	1.76	0.85
5:E:127:VAL:HG12	5:E:128:LYS:H	1.40	0.85
9:V:49:LEU:HD13	9:V:55:MET:HG2	1.57	0.85
2:B:51:ILE:HG12	2:B:204:MET:HG2	1.58	0.84
2:B:80:ALA:HA	2:B:84:ARG:HH12	1.42	0.84
2:B:209:ILE:HD13	2:B:378:LEU:HD23	1.60	0.84
3:C:342:GLN:HE21	3:C:343:PRO:HD2	1.43	0.84
2:O:209:ILE:HD13	2:O:378:LEU:HD23	1.60	0.84
2:O:248:ASN:HD22	2:O:248:ASN:C	1.81	0.83
5:E:121:GLN:HG2	5:E:170:ARG:CD	2.05	0.83
4:Q:47:ALA:H	4:Q:50:ASN:ND2	1.78	0.82
3:P:238:THR:HB	3:P:239:PRO:HD3	1.61	0.82
1:A:7:THR:HG21	2:B:113:ARG:HD2	1.62	0.82
3:P:342:GLN:HE21	3:P:343:PRO:HD2	1.45	0.82
2:O:160:LEU:HD12	9:V:64:LEU:HD13	1.62	0.81
1:N:331:ILE:HG21	1:N:431:LEU:HB2	1.61	0.81
3:C:9:HIS:HD2	3:C:12:LEU:H	1.26	0.81
2:B:27:THR:HG22	2:B:28:LYS:H	1.43	0.81
3:P:9:HIS:HD2	3:P:12:LEU:H	1.25	0.81
2:O:47:ILE:HD13	2:O:120:MET:HE2	1.62	0.81
1:A:106:MET:HG3	1:A:203:ILE:HD13	1.63	0.80
2:O:338:ARG:NH1	2:O:338:ARG:HG3	1.95	0.80
3:C:238:THR:HB	3:C:239:PRO:HD3	1.63	0.80
1:A:443:TRP:CE3	1:A:443:TRP:HA	2.17	0.79
3:P:69:HIS:CD2	3:P:73:ASN:HD22	1.99	0.79
1:N:37:VAL:HG12	1:N:199:ALA:HB1	1.63	0.79
3:C:22:LEU:HD21	14:C:2002:UQ:HM32	1.65	0.79
2:B:338:ARG:HG3	2:B:338:ARG:NH1	1.98	0.78
1:N:282:ARG:HH21	9:V:36:UNK:HA	1.48	0.78
2:B:248:ASN:HD22	2:B:248:ASN:C	1.85	0.78
2:B:37:SER:HB3	2:B:213:HIS:ND1	1.98	0.78
5:E:141:HIS:HB2	5:E:176:ALA:HB2	1.66	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:10:ASN:HD21	2:O:18:CYS:N	1.81	0.78
1:A:178:THR:HB	1:A:181:ASP:OD1	1.83	0.78
2:B:47:ILE:HD13	2:B:120:MET:CE	2.14	0.78
2:B:160:LEU:HD12	9:I:64:LEU:HD13	1.66	0.78
2:B:314:VAL:HG13	9:I:63:ASP:HB3	1.66	0.77
2:O:18:CYS:HB2	2:O:19:PRO:HD3	1.66	0.77
1:N:143:ASN:HD22	9:V:48:PRO:HD3	1.50	0.77
3:P:23:PRO:HG2	7:T:3:HIS:HB3	1.66	0.77
2:B:47:ILE:HD13	2:B:120:MET:HE2	1.66	0.77
1:A:331:ILE:HG21	1:A:431:LEU:HB2	1.67	0.77
2:B:31:ASN:ND2	2:B:31:ASN:H	1.83	0.77
4:D:47:ALA:H	4:D:50:ASN:ND2	1.82	0.77
5:E:119:ASP:HB3	5:E:179:ASN:HD21	1.48	0.77
2:B:76:THR:HG22	2:B:82:SER:N	1.99	0.76
5:E:121:GLN:CG	5:E:170:ARG:HD3	2.06	0.76
1:N:7:THR:HG21	2:O:113:ARG:HD2	1.65	0.76
1:N:443:TRP:CE3	1:N:443:TRP:HA	2.19	0.76
5:R:170:ARG:HA	5:R:179:ASN:HB3	1.67	0.76
3:P:212:ILE:HD12	6:S:62:ILE:HG23	1.67	0.76
2:O:76:THR:HG22	2:O:82:SER:N	1.99	0.76
5:E:81:ILE:HB	5:E:132:TRP:HH2	1.51	0.75
5:R:136:VAL:HG23	5:R:183:PRO:HD3	1.66	0.75
3:C:81:ARG:HH22	15:C:2011:GOL:H11	1.51	0.74
4:D:74:PRO:HB2	4:D:78:GLY:HA2	1.68	0.74
2:O:399:ALA:O	2:O:402:ILE:HG22	1.86	0.74
2:O:80:ALA:HA	2:O:84:ARG:HH12	1.52	0.74
1:A:298:ALA:HA	1:A:303:LEU:HB2	1.68	0.74
9:V:35:UNK:HG3	9:V:36:UNK:N	2.01	0.74
1:A:37:VAL:HG12	1:A:199:ALA:HB1	1.69	0.74
5:E:84:GLY:N	5:E:102:THR:HG23	2.02	0.74
4:Q:74:PRO:HB2	4:Q:78:GLY:HA2	1.70	0.74
3:C:69:HIS:CD2	3:C:73:ASN:HD22	2.04	0.74
9:I:34:UNK:HG3	9:I:35:UNK:N	2.03	0.74
2:B:341:MET:HE1	2:B:417:PHE:CE2	2.19	0.74
7:T:72:LYS:HE2	8:U:57:GLU:OE1	1.87	0.74
2:O:27:THR:HG22	2:O:28:LYS:N	2.03	0.74
2:B:399:ALA:O	2:B:402:ILE:HG22	1.86	0.74
1:A:443:TRP:HE3	1:A:443:TRP:HA	1.52	0.73
5:R:186:GLN:HE21	5:R:188:VAL:HG13	1.53	0.73
5:R:31:ASP:OD2	10:W:7:ARG:HG3	1.88	0.73
1:N:443:TRP:HE3	1:N:443:TRP:HA	1.53	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:ASP:OD2	9:I:33:UNK:HB2	1.88	0.73
3:C:23:PRO:HG2	7:G:3:HIS:HB3	1.68	0.73
1:N:298:ALA:HA	1:N:303:LEU:HB2	1.69	0.73
1:N:105:ASP:O	1:N:109:VAL:HG23	1.88	0.73
2:O:314:VAL:CG1	9:V:63:ASP:HB3	2.19	0.73
2:B:33:LEU:HD21	2:B:224:LEU:HD12	1.72	0.72
1:A:343:MET:HB3	1:A:444:ILE:HA	1.72	0.72
5:R:135:LEU:HD23	5:R:182:VAL:HG22	1.72	0.72
7:T:73:ASN:HD21	7:T:75:ALA:HB3	1.54	0.72
2:O:46:ARG:HG2	2:O:379:LEU:HD22	1.70	0.72
4:D:57:THR:HG22	4:D:59:ALA:N	2.04	0.72
2:O:62:ASN:O	2:O:65:THR:HG22	1.88	0.72
5:E:31:ASP:OD2	10:J:7:ARG:HG3	1.89	0.72
2:B:241:GLY:HA2	2:B:423:SER:HB3	1.71	0.72
2:O:217:LYS:O	2:O:221:GLU:HG2	1.90	0.72
5:E:86:ASN:OD1	5:E:99:ARG:HB2	1.90	0.71
4:Q:231:LYS:O	6:S:71:LYS:HE3	1.91	0.71
2:B:27:THR:HG22	2:B:28:LYS:N	2.03	0.71
7:T:80:ASP:HB3	8:U:47:ARG:HH11	1.55	0.71
5:E:166:ASP:OD2	5:E:170:ARG:HB2	1.90	0.71
1:N:37:VAL:HG12	1:N:199:ALA:CB	2.19	0.71
2:B:31:ASN:HD22	2:B:31:ASN:H	1.37	0.71
2:B:38:LEU:HD12	2:B:39:GLU:N	2.06	0.71
1:N:111:GLU:HG3	1:N:215:HIS:CD2	2.25	0.71
2:O:181:TYR:CE1	2:O:182:ARG:HG3	2.26	0.71
1:A:103:SER:HB3	1:A:202:GLY:O	1.90	0.71
1:N:182:LEU:O	1:N:186:ILE:HG13	1.91	0.71
6:S:91:GLU:O	6:S:95:LYS:HG3	1.91	0.71
1:A:336:PHE:CZ	3:C:4:ASN:HB3	2.26	0.71
4:D:62:LYS:O	4:D:66:GLU:HG3	1.91	0.71
2:B:76:THR:CG2	2:B:82:SER:H	2.00	0.70
2:O:206:LEU:HD23	2:O:220:ALA:HB2	1.73	0.70
9:I:70:LEU:HD23	9:I:71:ASN:H	1.56	0.70
2:O:154:SER:O	2:O:157:VAL:HG12	1.91	0.70
1:N:242:ARG:HH12	1:N:432:LEU:HA	1.55	0.70
3:P:247:SER:OG	3:P:250:LEU:HB2	1.92	0.70
3:P:301:ILE:HD11	3:P:364:LEU:HD21	1.74	0.70
1:N:178:THR:HB	1:N:181:ASP:OD1	1.89	0.70
2:O:221:GLU:HG3	2:O:222:GLN:H	1.57	0.70
2:B:31:ASN:N	2:B:31:ASN:HD22	1.90	0.70
1:A:282:ARG:HH21	9:I:35:UNK:HA	1.57	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:47:ILE:HD13	2:O:120:MET:CE	2.21	0.70
2:B:46:ARG:HG2	2:B:379:LEU:HD22	1.73	0.69
10:J:7:ARG:NH1	10:J:7:ARG:HB3	2.07	0.69
1:A:60:GLU:OE2	1:A:90:THR:HG22	1.91	0.69
1:A:242:ARG:HH12	1:A:432:LEU:HA	1.57	0.69
1:A:281:ASP:CG	9:I:33:UNK:HB2	2.13	0.69
5:E:76:ILE:HD13	5:E:98:VAL:HG21	1.74	0.69
8:H:10:GLU:O	8:H:11:GLU:HG3	1.92	0.69
5:E:30:GLU:HB2	10:J:7:ARG:HG2	1.74	0.69
2:O:128:THR:HG21	2:O:224:LEU:HD22	1.75	0.69
2:O:361:LYS:O	2:O:365:LYS:HG3	1.93	0.69
2:B:80:ALA:HA	2:B:84:ARG:NH1	2.07	0.69
8:U:28:GLU:HG2	8:U:32:LYS:HE3	1.75	0.68
2:B:181:TYR:CE1	2:B:182:ARG:HG3	2.28	0.68
3:C:41:CYS:HG	3:C:90:PHE:HD2	1.41	0.68
2:O:225:ASN:O	2:O:227:ARG:HG3	1.93	0.68
5:R:30:GLU:HB2	10:W:7:ARG:HG2	1.76	0.68
1:N:402:VAL:HG22	1:N:406:MET:CE	2.23	0.68
1:A:37:VAL:HG12	1:A:199:ALA:CB	2.24	0.68
5:E:83:GLU:HB3	5:E:102:THR:HG22	1.73	0.68
5:E:86:ASN:HB2	5:E:99:ARG:HE	1.59	0.68
5:R:109:GLU:CG	5:R:123:ASP:HB2	2.23	0.68
8:U:27:THR:O	8:U:31:VAL:HG23	1.94	0.68
1:A:336:PHE:CE2	3:C:4:ASN:HB3	2.29	0.68
2:B:124:LEU:HD11	2:B:223:PHE:CB	2.23	0.68
4:Q:26:VAL:HG12	4:Q:55:THR:HG21	1.75	0.68
4:D:231:LYS:O	6:F:71:LYS:HE3	1.93	0.68
1:N:85:HIS:CD2	2:O:284:LEU:HD22	2.28	0.68
5:R:119:ASP:HB3	5:R:179:ASN:ND2	2.09	0.67
5:R:83:GLU:HB3	5:R:102:THR:HG22	1.75	0.67
2:O:341:MET:HE2	2:O:341:MET:HA	1.74	0.67
3:P:37:LEU:HD21	3:P:233:LEU:HA	1.76	0.67
3:P:106:GLY:HA2	3:P:108:TYR:CE2	2.29	0.67
4:Q:62:LYS:O	4:Q:66:GLU:HG3	1.94	0.67
5:R:78:LEU:HB3	5:R:132:TRP:CZ2	2.30	0.67
5:R:134:ILE:HD12	5:R:185:TYR:CD1	2.29	0.67
5:E:122:HIS:HB3	5:E:125:ASP:CG	2.14	0.67
5:R:102:THR:O	5:R:106:ILE:HG13	1.94	0.67
2:B:154:SER:O	2:B:157:VAL:HG12	1.95	0.67
5:R:166:ASP:OD2	5:R:170:ARG:HB2	1.95	0.67
5:E:127:VAL:HG12	5:E:128:LYS:N	2.08	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:60:GLU:OE2	1:N:90:THR:HG22	1.95	0.67
3:C:37:LEU:HD21	3:C:233:LEU:HA	1.76	0.66
4:Q:57:THR:HG22	4:Q:59:ALA:N	2.10	0.66
1:A:350:THR:HG22	1:A:352:SER:H	1.60	0.66
9:V:28:UNK:CB	9:V:72:ALA:HB2	2.25	0.66
2:O:357:VAL:HG12	2:O:361:LYS:HE3	1.76	0.66
3:P:41:CYS:HG	3:P:90:PHE:HD2	1.43	0.66
2:B:394:ALA:HB3	2:B:397:VAL:HG23	1.77	0.66
3:C:377:MET:HE2	6:F:20:TYR:HB2	1.78	0.66
2:O:169:LYS:HG3	2:O:240:TRP:HB2	1.76	0.66
2:B:299:VAL:HG11	2:B:336:VAL:HG13	1.77	0.66
5:R:78:LEU:HD13	5:R:132:TRP:NE1	2.10	0.66
5:E:52:LYS:C	5:E:52:LYS:HD3	2.15	0.66
10:W:7:ARG:HB3	10:W:7:ARG:NH1	2.10	0.66
5:E:129:LYS:HB3	5:E:132:TRP:HB2	1.78	0.65
2:O:394:ALA:HB3	2:O:397:VAL:HG23	1.78	0.65
5:R:81:ILE:HG22	5:R:100:HIS:HB2	1.76	0.65
5:E:130:PRO:HG2	5:E:131:GLU:CD	2.17	0.65
1:N:112:LEU:O	1:N:116:VAL:HG23	1.96	0.65
5:R:83:GLU:HA	5:R:100:HIS:HB3	1.77	0.65
1:A:69:LYS:HD2	1:A:70:ARG:HH21	1.61	0.65
2:B:306:PRO:HA	9:I:52:ARG:CG	2.26	0.65
5:E:130:PRO:HG2	5:E:131:GLU:H	1.61	0.65
1:N:39:VAL:HG11	1:N:117:VAL:HG11	1.77	0.65
2:O:299:VAL:HG11	2:O:336:VAL:HG13	1.76	0.65
7:T:36:ASN:OD1	7:T:39:ARG:NH1	2.30	0.65
4:D:235:MET:HB3	7:G:15:THR:HG22	1.78	0.65
5:E:190:ASP:C	5:E:192:LEU:H	1.98	0.65
8:H:28:GLU:HG2	8:H:32:LYS:HE3	1.77	0.65
3:C:301:ILE:HD11	3:C:364:LEU:HD21	1.78	0.65
1:N:336:PHE:CZ	3:P:4:ASN:HB3	2.32	0.65
2:O:150:VAL:O	2:O:153:GLN:HG3	1.97	0.65
2:O:422:LYS:O	2:O:436:LEU:HD21	1.95	0.65
3:C:106:GLY:HA2	3:C:108:TYR:CE2	2.31	0.64
1:N:69:LYS:HD2	1:N:70:ARG:HH21	1.63	0.64
2:O:341:MET:HE1	2:O:417:PHE:CE2	2.27	0.64
4:Q:235:MET:HB3	7:T:15:THR:HG22	1.78	0.64
2:B:270:ASN:ND2	2:B:270:ASN:H	1.94	0.64
3:C:212:ILE:HD12	6:F:62:ILE:HG23	1.79	0.64
6:S:53:ASP:OD1	6:S:54:LEU:N	2.30	0.64
1:A:282:ARG:NH2	9:I:35:UNK:HA	2.12	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:119:ASP:HB3	5:E:179:ASN:ND2	2.12	0.64
8:H:27:THR:O	8:H:31:VAL:HG23	1.97	0.64
2:O:353:THR:HG22	2:O:355:GLU:N	2.00	0.64
5:R:86:ASN:OD1	5:R:99:ARG:HB2	1.97	0.64
3:C:49:GLY:C	12:C:501:HEM:HAC	2.17	0.64
2:O:286:LYS:HE2	2:O:287:ARG:NH1	2.12	0.64
2:B:63:LEU:HB2	2:B:182:ARG:HD3	1.79	0.64
2:O:80:ALA:HA	2:O:84:ARG:NH1	2.12	0.64
1:A:111:GLU:HG3	1:A:215:HIS:CD2	2.33	0.64
2:B:422:LYS:O	2:B:436:LEU:HD21	1.98	0.64
6:F:53:ASP:OD1	6:F:54:LEU:N	2.30	0.64
3:P:25:PRO:HB2	3:P:28:ILE:HG23	1.78	0.64
3:C:342:GLN:NE2	3:C:343:PRO:HD2	2.13	0.64
7:G:36:ASN:OD1	7:G:39:ARG:NH1	2.31	0.64
1:N:282:ARG:NH2	9:V:37:UNK:N	2.45	0.64
1:N:350:THR:HG22	1:N:352:SER:H	1.62	0.64
1:A:182:LEU:O	1:A:186:ILE:HG13	1.98	0.64
5:R:52:LYS:HD3	5:R:52:LYS:C	2.18	0.64
2:B:46:ARG:HD2	2:B:110:GLU:CG	2.28	0.63
3:C:247:SER:OG	3:C:250:LEU:HB2	1.99	0.63
2:O:63:LEU:HB2	2:O:182:ARG:HD3	1.79	0.63
8:H:28:GLU:O	8:H:32:LYS:HG3	1.97	0.63
1:N:143:ASN:HD22	9:V:48:PRO:CD	2.11	0.63
2:O:192:HIS:O	2:O:196:GLN:HG3	1.98	0.63
8:U:43:ARG:O	8:U:47:ARG:HG3	1.97	0.63
3:C:25:PRO:HB2	3:C:28:ILE:HG23	1.81	0.63
5:R:86:ASN:HB2	5:R:99:ARG:HE	1.63	0.63
2:B:341:MET:HE2	2:B:341:MET:HA	1.81	0.63
2:O:219:VAL:O	2:O:223:PHE:HB2	1.98	0.63
6:S:91:GLU:HG2	6:S:95:LYS:HE3	1.80	0.63
7:T:79:ASN:O	7:T:80:ASP:HB2	1.97	0.63
2:B:306:PRO:HA	9:I:52:ARG:HG2	1.80	0.63
4:D:26:VAL:HG12	4:D:55:THR:HG21	1.80	0.63
1:N:343:MET:HB3	1:N:444:ILE:HA	1.81	0.63
2:O:241:GLY:HA2	2:O:423:SER:HB3	1.81	0.63
2:B:341:MET:HA	2:B:341:MET:CE	2.29	0.62
1:N:15:ASN:O	1:N:26:ALA:HA	1.98	0.62
1:A:39:VAL:HG11	1:A:117:VAL:HG11	1.80	0.62
1:A:85:HIS:CD2	2:B:284:LEU:HD22	2.34	0.62
10:J:7:ARG:HH11	10:J:7:ARG:CB	2.11	0.62
5:R:109:GLU:HG2	5:R:123:ASP:HB2	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:78:LEU:HD11	5:R:187:PHE:CD1	2.33	0.62
2:B:150:VAL:O	2:B:153:GLN:HG3	1.99	0.62
1:N:233:ARG:HH21	1:N:316:ASP:HB2	1.64	0.62
2:O:207:VAL:HG12	2:O:208:GLY:H	1.64	0.62
2:O:273:SER:O	2:O:276:GLN:HB3	1.99	0.62
3:P:101:ARG:C	3:P:101:ARG:HD2	2.20	0.62
3:P:342:GLN:NE2	3:P:343:PRO:HD2	2.14	0.62
3:C:236:MET:O	3:C:239:PRO:HD2	1.99	0.62
2:B:361:LYS:O	2:B:365:LYS:HG3	2.00	0.62
5:E:129:LYS:CB	5:E:132:TRP:HB2	2.29	0.62
2:O:47:ILE:HG21	2:O:120:MET:HE1	1.80	0.62
3:P:49:GLY:C	12:P:501:HEM:HAC	2.19	0.62
6:F:42:ASP:OD1	6:F:101:ARG:NH1	2.32	0.62
5:E:55:VAL:O	5:E:59:ILE:HG12	2.00	0.62
2:B:207:VAL:HG12	2:B:208:GLY:H	1.64	0.62
3:P:22:LEU:HD21	14:P:3002:UQ:HM32	1.81	0.62
2:B:357:VAL:HG12	2:B:361:LYS:HE3	1.80	0.62
5:E:101:ARG:HA	5:E:105:GLU:OE1	1.99	0.62
2:O:38:LEU:HD12	2:O:39:GLU:N	2.15	0.62
3:P:377:MET:HE2	6:S:20:TYR:HB2	1.82	0.62
5:E:81:ILE:HB	5:E:132:TRP:CH2	2.34	0.61
7:G:73:ASN:HD21	7:G:75:ALA:HB3	1.64	0.61
5:E:147:ILE:O	5:E:156:TYR:HA	1.99	0.61
3:C:328:LEU:CD1	7:G:51:PRO:HB3	2.24	0.61
2:B:62:ASN:O	2:B:65:THR:HG22	2.00	0.61
1:N:106:MET:O	1:N:110:VAL:HG23	2.00	0.61
2:O:46:ARG:HD2	2:O:110:GLU:CG	2.30	0.61
2:B:201:SER:OG	2:B:228:SER:HA	1.99	0.61
5:E:106:ILE:C	5:E:110:ALA:HB3	2.20	0.61
2:O:22:GLU:HG2	2:O:39:GLU:HB3	1.82	0.61
3:P:236:MET:O	3:P:239:PRO:HD2	2.00	0.61
2:B:47:ILE:HG21	2:B:120:MET:HE1	1.83	0.61
2:B:207:VAL:HG21	2:B:383:GLY:HA3	1.83	0.61
3:C:37:LEU:O	3:C:41:CYS:HB2	2.01	0.61
4:D:75:ASP:OD2	4:D:79:GLU:HB2	2.00	0.61
5:E:136:VAL:CG2	5:E:183:PRO:HD3	2.28	0.61
1:N:336:PHE:CE2	3:P:4:ASN:HB3	2.36	0.60
8:U:28:GLU:O	8:U:32:LYS:HG3	2.01	0.60
5:E:78:LEU:HD12	5:E:190:ASP:O	2.01	0.60
4:Q:76:GLU:CD	4:Q:76:GLU:H	2.05	0.60
5:R:83:GLU:HG3	5:R:100:HIS:CE1	2.36	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:VAL:HG22	1:A:406:MET:CE	2.32	0.60
7:T:73:ASN:ND2	7:T:75:ALA:HB3	2.17	0.60
2:O:397:VAL:O	2:O:401:LYS:HG2	2.02	0.60
3:P:146:VAL:HG21	3:P:269:ILE:HG21	1.83	0.60
5:R:171:ILE:HG22	5:R:179:ASN:OD1	2.00	0.60
3:C:146:VAL:HG21	3:C:269:ILE:HG21	1.84	0.60
1:N:170:THR:HG22	1:N:171:THR:N	2.16	0.60
9:I:31:UNK:C	9:I:73:PRO:HG2	2.31	0.60
7:T:50:PRO:HB2	7:T:51:PRO:CD	2.31	0.60
5:R:117:LEU:HD21	5:R:172:ARG:NH1	2.17	0.60
2:B:192:HIS:O	2:B:196:GLN:HG3	2.01	0.60
2:B:299:VAL:CG1	2:B:336:VAL:HG13	2.31	0.60
2:O:76:THR:HG23	2:O:136:GLU:OE1	2.01	0.60
1:N:85:HIS:NE2	2:O:284:LEU:HD22	2.17	0.60
2:O:341:MET:HA	2:O:341:MET:CE	2.31	0.60
2:B:202:ALA:HB3	2:B:229:GLY:O	2.02	0.60
10:W:7:ARG:HH11	10:W:7:ARG:CB	2.15	0.60
2:O:18:CYS:HB2	2:O:19:PRO:CD	2.32	0.59
2:O:248:ASN:C	2:O:248:ASN:ND2	2.55	0.59
2:O:299:VAL:CG1	2:O:336:VAL:HG13	2.32	0.59
1:A:15:ASN:O	1:A:26:ALA:HA	2.02	0.59
5:E:122:HIS:HE1	5:E:124:LEU:HD12	1.66	0.59
1:N:136:GLN:OE1	9:V:50:LEU:HB3	2.03	0.59
1:N:395:TRP:HA	1:N:395:TRP:CE3	2.37	0.59
3:P:37:LEU:O	3:P:41:CYS:HB2	2.02	0.59
1:A:186:ILE:HG23	1:A:190:PHE:CD1	2.37	0.59
2:O:248:ASN:HD21	2:O:250:HIS:HB2	1.68	0.59
16:Q:501:HEC:HMB1	16:Q:501:HEC:HBB3	1.85	0.59
5:E:101:ARG:HB2	5:E:131:GLU:HA	1.82	0.59
2:O:144:LEU:HB2	2:O:183:ILE:HD12	1.84	0.59
2:O:372:VAL:O	2:O:372:VAL:HG12	2.02	0.59
4:Q:75:ASP:OD2	4:Q:79:GLU:HB2	2.02	0.59
2:B:144:LEU:HB2	2:B:183:ILE:HD12	1.84	0.59
2:O:76:THR:CG2	2:O:82:SER:H	2.04	0.59
5:E:171:ILE:HG22	5:E:179:ASN:OD1	2.03	0.59
6:S:42:ASP:OD1	6:S:101:ARG:NH1	2.36	0.59
6:S:11:ARG:HA	6:S:14:ASP:HB2	1.85	0.59
1:A:105:ASP:O	1:A:109:VAL:HG23	2.03	0.58
3:C:245:LEU:O	4:D:201:ARG:HD2	2.02	0.58
3:P:199:THR:HA	18:P:2010:BOG:O1	2.03	0.58
4:Q:12:TRP:NE1	4:Q:125:ASP:OD2	2.31	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:TYR:CG	1:A:281:ASP:N	2.71	0.58
8:H:40:CYS:O	8:H:44:VAL:HG23	2.03	0.58
5:E:106:ILE:O	5:E:110:ALA:HB3	2.03	0.58
2:O:124:LEU:HD11	2:O:223:PHE:HB3	1.84	0.58
5:R:186:GLN:NE2	5:R:188:VAL:HG13	2.17	0.58
1:A:49:ASN:HD21	1:A:51:LYS:HE3	1.69	0.58
2:B:57:TYR:CE2	2:B:203:ARG:NH2	2.70	0.58
2:B:33:LEU:CD2	2:B:224:LEU:HD12	2.32	0.58
9:I:70:LEU:HD23	9:I:71:ASN:N	2.19	0.58
2:B:169:LYS:HG3	2:B:240:TRP:HB2	1.84	0.58
1:N:69:LYS:HD2	1:N:70:ARG:NH2	2.18	0.58
8:U:27:THR:HG22	8:U:29:LYS:H	1.66	0.58
4:D:97:ASN:HB2	4:D:98:PRO:HD2	1.85	0.58
5:E:114:VAL:HG21	5:E:172:ARG:NH1	2.19	0.58
5:R:45:VAL:HG13	10:W:28:ALA:HA	1.86	0.58
2:B:207:VAL:HG12	2:B:208:GLY:N	2.19	0.58
2:O:101:THR:HG23	2:O:104:LYS:HE3	1.85	0.58
2:B:248:ASN:HD21	2:B:250:HIS:HB2	1.69	0.58
4:D:167:GLU:HG3	8:H:13:LEU:CD2	2.34	0.58
5:E:163:SER:HA	5:E:174:GLY:HA3	1.86	0.58
2:O:57:TYR:CE2	2:O:203:ARG:NH2	2.71	0.58
1:A:69:LYS:HD2	1:A:70:ARG:NH2	2.18	0.57
2:B:276:GLN:HG2	2:B:281:ALA:HB2	1.86	0.57
1:N:178:THR:HG22	1:N:180:ALA:N	2.08	0.57
4:Q:139:ALA:HB3	8:U:54:CYS:SG	2.44	0.57
1:A:178:THR:CG2	1:A:179:ARG:N	2.67	0.57
2:B:372:VAL:O	2:B:372:VAL:HG12	2.04	0.57
1:N:173:ASN:O	1:N:177:LEU:HG	2.04	0.57
1:N:371:GLY:O	1:N:375:VAL:HG23	2.05	0.57
1:N:331:ILE:CG2	1:N:431:LEU:HB2	2.34	0.57
6:S:99:ARG:HB3	6:S:99:ARG:NH1	2.20	0.57
1:A:131:ARG:NH2	1:A:177:LEU:O	2.37	0.57
6:F:73:ARG:NH1	7:G:32:ASP:OD2	2.37	0.57
2:O:27:THR:CG2	2:O:28:LYS:H	2.11	0.57
9:V:65:VAL:HG12	9:V:66:ALA:N	2.19	0.57
1:A:85:HIS:NE2	2:B:284:LEU:HD22	2.20	0.57
5:E:109:GLU:OE2	5:E:153:PHE:HB3	2.03	0.57
3:C:9:HIS:CD2	3:C:12:LEU:H	2.15	0.57
9:V:70:LEU:HD23	9:V:71:ASN:N	2.20	0.57
2:O:334:GLY:O	2:O:338:ARG:HG2	2.05	0.57
1:N:317:THR:HG23	1:N:318:GLY:N	2.19	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:47:ILE:HD11	2:O:116:VAL:HG13	1.87	0.57
2:O:318:ASP:O	2:O:319:SER:HB2	2.05	0.57
7:G:49:ALA:HB3	7:G:50:PRO:HD3	1.87	0.57
5:R:163:SER:H	5:R:175:PRO:HD2	1.70	0.57
1:A:130:GLU:O	1:A:134:ILE:HG13	2.04	0.56
4:D:229:VAL:HG23	7:G:20:PRO:HG3	1.85	0.56
1:N:37:VAL:HG23	1:N:113:LEU:HD11	1.87	0.56
5:R:134:ILE:HD12	5:R:185:TYR:CE1	2.39	0.56
5:R:188:VAL:HG23	5:R:192:LEU:HB2	1.86	0.56
2:B:24:LEU:HD12	2:B:37:SER:O	2.05	0.56
2:O:407:SER:O	2:O:411:VAL:HG23	2.05	0.56
2:O:357:VAL:O	2:O:361:LYS:HG3	2.05	0.56
3:P:153:ALA:HB2	3:P:288:LYS:HG2	1.87	0.56
1:A:106:MET:O	1:A:110:VAL:HG23	2.04	0.56
1:A:395:TRP:HA	1:A:395:TRP:CE3	2.40	0.56
1:N:178:THR:CG2	1:N:179:ARG:N	2.67	0.56
3:P:9:HIS:CD2	3:P:12:LEU:H	2.15	0.56
1:N:10:ASN:HD21	2:O:19:PRO:HD2	1.70	0.56
6:S:17:ARG:HG2	6:S:17:ARG:HH11	1.71	0.56
2:B:225:ASN:O	2:B:227:ARG:N	2.38	0.56
11:P:3007:PEE:H50	17:T:3004:CDL:H712	1.88	0.56
2:B:46:ARG:NH2	2:B:376:GLN:HG3	2.20	0.56
5:E:45:VAL:HG13	10:J:28:ALA:HA	1.87	0.56
5:R:161:HIS:HB2	5:R:175:PRO:HG3	1.88	0.56
8:U:21:ARG:HG3	8:U:21:ARG:HH11	1.69	0.56
2:B:206:LEU:HD23	2:B:220:ALA:HB2	1.87	0.56
7:G:40:ARG:HB3	17:G:2004:CDL:HA32	1.86	0.56
1:A:196:VAL:HG11	1:A:383:LEU:HD12	1.87	0.56
1:N:131:ARG:NH2	1:N:177:LEU:O	2.37	0.56
2:O:31:ASN:H	2:O:31:ASN:ND2	2.04	0.56
1:A:178:THR:HG22	1:A:180:ALA:N	2.07	0.56
1:N:103:SER:HB3	1:N:202:GLY:O	2.06	0.56
1:N:18:THR:HG23	1:N:24:ARG:HG3	1.88	0.56
1:A:17:THR:HG23	1:A:205:HIS:NE2	2.21	0.55
2:B:71:LEU:HD12	2:B:144:LEU:HD23	1.87	0.55
2:O:221:GLU:C	2:O:223:PHE:H	2.10	0.55
2:O:207:VAL:HG21	2:O:383:GLY:HA3	1.89	0.55
5:R:73:LYS:HB3	5:R:196:GLY:O	2.05	0.55
7:T:72:LYS:CE	8:U:57:GLU:OE1	2.53	0.55
1:A:7:THR:HG21	2:B:113:ARG:CD	2.32	0.55
2:B:122:TYR:O	2:B:126:VAL:HG23	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:135:LEU:HD11	5:E:169:GLY:HA3	1.89	0.55
10:W:49:GLY:N	10:W:54:HIS:ND1	2.54	0.55
5:E:116:LYS:HD2	5:E:116:LYS:N	2.22	0.55
7:G:50:PRO:HB2	7:G:51:PRO:CD	2.36	0.55
1:N:130:GLU:O	1:N:134:ILE:HG13	2.07	0.55
1:A:64:PHE:HE2	1:A:86:PHE:CZ	2.25	0.55
7:G:41:PHE:CE2	7:G:45:VAL:HG21	2.41	0.55
2:O:207:VAL:HG12	2:O:208:GLY:N	2.22	0.55
2:O:402:ILE:HD13	2:O:402:ILE:C	2.27	0.55
1:A:369:LEU:HD12	1:A:392:LEU:HD11	1.89	0.55
4:D:102:ARG:HG2	4:D:102:ARG:HH11	1.71	0.55
5:E:131:GLU:H	5:E:131:GLU:CD	2.10	0.55
5:R:55:VAL:O	5:R:59:ILE:HG12	2.06	0.55
2:O:156:GLN:HE22	9:V:77:ARG:C	2.09	0.55
1:A:106:MET:O	1:A:106:MET:HE2	2.07	0.55
3:P:69:HIS:HD2	3:P:73:ASN:HD22	1.50	0.55
5:R:81:ILE:HG12	5:R:87:VAL:HG21	1.87	0.55
3:P:313:GLN:NE2	6:S:36:THR:OG1	2.40	0.55
4:Q:229:VAL:HG23	7:T:20:PRO:HG3	1.89	0.55
1:A:170:THR:HG22	1:A:171:THR:N	2.23	0.55
2:O:56:ARG:HH12	2:O:172:LEU:HG	1.72	0.55
2:O:221:GLU:O	2:O:223:PHE:N	2.40	0.55
5:R:99:ARG:HB3	5:R:133:VAL:CG1	2.37	0.55
9:I:65:VAL:HG12	9:I:66:ALA:N	2.22	0.54
2:O:71:LEU:HD12	2:O:144:LEU:HD23	1.89	0.54
2:B:397:VAL:O	2:B:401:LYS:HG2	2.07	0.54
5:E:84:GLY:CA	5:E:102:THR:HG23	2.37	0.54
5:E:99:ARG:HD3	5:E:105:GLU:OE2	2.08	0.54
10:J:7:ARG:HB3	10:J:7:ARG:HH11	1.72	0.54
1:A:4:TYR:HB3	2:B:114:ASP:OD2	2.07	0.54
2:O:56:ARG:HG3	2:O:56:ARG:HH11	1.71	0.54
1:A:23:LEU:HD23	1:A:24:ARG:N	2.22	0.54
2:B:264:VAL:HG23	2:B:316:TYR:C	2.28	0.54
2:B:357:VAL:O	2:B:361:LYS:HG3	2.06	0.54
1:N:187:ASP:O	1:N:191:LYS:HE3	2.07	0.54
2:O:24:LEU:HD12	2:O:37:SER:O	2.08	0.54
17:Q:3003:CDL:HB22	7:T:40:ARG:NH2	2.22	0.54
5:R:49:TYR:CE1	10:W:32:GLU:HG3	2.43	0.54
2:B:96:LEU:H	9:I:70:LEU:HD22	1.72	0.54
2:O:59:THR:HG22	2:O:61:ALA:H	1.73	0.54
1:A:191:LYS:CA	1:A:195:MET:HE2	2.38	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:195:GLU:OE1	4:D:201:ARG:NH2	2.41	0.54
5:E:130:PRO:HG2	5:E:131:GLU:OE1	2.06	0.54
3:P:202:HIS:NE2	14:P:3002:UQ:O4	2.36	0.54
3:C:150:LEU:HB3	3:C:292:VAL:HG22	1.90	0.54
8:H:18:THR:O	8:H:22:GLU:HG3	2.08	0.54
2:O:140:LEU:O	2:O:143:GLN:HB3	2.07	0.54
1:A:288:LYS:HE3	1:A:289:HIS:CE1	2.43	0.54
1:N:295:ALA:O	1:N:299:VAL:HG23	2.08	0.54
1:N:4:TYR:HB3	2:O:114:ASP:OD2	2.08	0.54
2:O:276:GLN:HG2	2:O:281:ALA:HB2	1.90	0.54
2:O:31:ASN:N	2:O:31:ASN:HD22	2.06	0.54
7:T:50:PRO:HB2	7:T:51:PRO:HD3	1.90	0.54
8:U:28:GLU:CG	8:U:32:LYS:HE3	2.38	0.54
2:B:56:ARG:HH12	2:B:172:LEU:HG	1.72	0.54
2:B:212:LYS:HB3	2:B:215:ASP:OD2	2.08	0.54
3:P:245:LEU:O	4:Q:201:ARG:HD2	2.08	0.54
7:G:72:LYS:HE2	8:H:57:GLU:OE1	2.07	0.54
5:R:78:LEU:HD11	5:R:187:PHE:CE1	2.43	0.54
7:T:41:PHE:CE2	7:T:45:VAL:HG21	2.44	0.53
9:V:70:LEU:HD23	9:V:71:ASN:OD1	2.08	0.53
2:B:286:LYS:HE2	2:B:287:ARG:NH1	2.23	0.53
1:N:49:ASN:ND2	1:N:51:LYS:H	2.04	0.53
7:T:40:ARG:HB3	17:T:3004:CDL:HA32	1.89	0.53
3:C:263:LEU:O	3:C:264:VAL:HG23	2.08	0.53
3:C:325:LEU:HD21	3:C:366:LEU:HB3	1.89	0.53
5:E:83:GLU:HB3	5:E:102:THR:CG2	2.38	0.53
10:J:56:LYS:O	10:J:60:GLU:HB2	2.09	0.53
1:N:186:ILE:HG23	1:N:190:PHE:CD1	2.43	0.53
3:P:121:LEU:O	3:P:125:MET:HG3	2.07	0.53
2:B:248:ASN:ND2	2:B:248:ASN:C	2.58	0.53
2:B:47:ILE:HD13	2:B:120:MET:HE1	1.90	0.53
1:N:369:LEU:HD12	1:N:392:LEU:HD11	1.89	0.53
4:Q:97:ASN:HB2	4:Q:98:PRO:HD2	1.89	0.53
4:Q:237:TYR:HB2	6:S:60:PHE:CG	2.43	0.53
2:B:133:ARG:HD3	2:B:135:TRP:CZ2	2.44	0.53
12:C:502:HEM:HMC2	12:C:502:HEM:HBC2	1.89	0.53
5:R:77:LYS:HA	5:R:191:ASP:O	2.09	0.53
2:B:75:LEU:HD22	2:B:136:GLU:HB3	1.90	0.53
2:B:34:ILE:HD13	2:B:390:GLY:HA2	1.90	0.53
3:C:334:LEU:HD21	11:C:2007:PEE:H65	1.89	0.53
6:F:11:ARG:O	6:F:15:ARG:HG3	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:196:VAL:HG11	1:N:383:LEU:HD12	1.90	0.53
1:N:35:CYS:SG	1:N:203:ILE:HD11	2.48	0.53
4:D:47:ALA:HA	4:D:90:TYR:HA	1.90	0.53
5:E:135:LEU:HD23	5:E:182:VAL:HG22	1.91	0.53
3:P:150:LEU:HB3	3:P:292:VAL:HG22	1.90	0.53
6:S:73:ARG:NH1	7:T:32:ASP:OD2	2.42	0.53
8:H:27:THR:HG22	8:H:29:LYS:H	1.74	0.53
2:B:273:SER:O	2:B:276:GLN:HB3	2.08	0.53
4:D:102:ARG:HA	4:D:108:ALA:O	2.08	0.53
9:I:29:UNK:O	9:I:30:UNK:HB2	2.08	0.53
10:J:49:GLY:N	10:J:54:HIS:ND1	2.57	0.53
1:N:49:ASN:HD21	1:N:51:LYS:HE3	1.73	0.53
2:B:101:THR:HG23	2:B:104:LYS:HE3	1.90	0.52
2:B:21:ALA:O	2:B:22:GLU:HB3	2.08	0.52
7:T:80:ASP:HB3	8:U:47:ARG:NH1	2.24	0.52
2:B:140:LEU:O	2:B:143:GLN:HB3	2.08	0.52
2:B:153:GLN:HE22	9:I:34:UNK:CG	2.22	0.52
3:C:28:ILE:HG12	3:C:225:TYR:OH	2.09	0.52
4:D:79:GLU:HA	4:D:79:GLU:OE2	2.09	0.52
1:N:64:PHE:HE2	1:N:86:PHE:CZ	2.27	0.52
2:O:72:ALA:HB1	2:O:75:LEU:HD12	1.92	0.52
2:B:318:ASP:O	2:B:319:SER:HB2	2.09	0.52
2:O:46:ARG:NH2	2:O:376:GLN:HG3	2.24	0.52
3:P:28:ILE:HG12	3:P:225:TYR:OH	2.09	0.52
3:P:78:TRP:CZ3	4:Q:201:ARG:HG3	2.44	0.52
1:A:268:VAL:O	1:A:272:VAL:HG23	2.10	0.52
7:G:65:GLU:O	7:G:69:LEU:HG	2.09	0.52
9:I:38:UNK:O	9:I:39:UNK:C	2.56	0.52
1:N:26:ALA:HB2	1:N:383:LEU:HD11	1.92	0.52
2:O:34:ILE:HD13	2:O:390:GLY:HA2	1.91	0.52
3:P:138:GLN:HB2	3:P:255:GLU:O	2.10	0.52
5:R:188:VAL:HG23	5:R:192:LEU:CB	2.40	0.52
6:S:40:ASP:O	6:S:44:LYS:HG3	2.10	0.52
4:Q:134:TYR:CG	4:Q:162:PRO:HG3	2.45	0.52
2:B:59:THR:HG22	2:B:60:THR:N	2.25	0.52
4:D:26:VAL:HG22	4:D:188:THR:HG22	1.92	0.52
10:J:60:GLU:HA	10:J:60:GLU:OE2	2.10	0.52
2:O:338:ARG:NH1	2:O:338:ARG:CG	2.67	0.52
5:R:178:TYR:N	5:R:178:TYR:CD1	2.78	0.52
8:U:18:THR:O	8:U:22:GLU:HG3	2.10	0.52
2:B:402:ILE:HD13	2:B:402:ILE:C	2.30	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:178:TYR:H	5:E:178:TYR:HD1	1.58	0.52
5:E:76:ILE:CD1	5:E:98:VAL:HG21	2.37	0.52
5:E:187:PHE:C	5:E:189:GLY:H	2.13	0.52
6:S:99:ARG:HB3	6:S:99:ARG:HH11	1.75	0.52
1:A:37:VAL:HG23	1:A:113:LEU:HD11	1.90	0.51
2:B:27:THR:CG2	2:B:28:LYS:H	2.17	0.51
2:B:334:GLY:O	2:B:338:ARG:HG2	2.10	0.51
2:O:259:THR:HG22	2:O:260:GLU:N	2.24	0.51
2:O:361:LYS:HA	2:O:402:ILE:HD11	1.91	0.51
4:Q:70:VAL:HG21	4:Q:83:ARG:CZ	2.40	0.51
4:Q:229:VAL:CG2	7:T:20:PRO:HG3	2.40	0.51
2:B:189:GLU:OE1	2:B:189:GLU:N	2.42	0.51
3:C:69:HIS:HD2	3:C:73:ASN:HD22	1.55	0.51
5:E:146:PRO:HG2	5:E:180:LEU:HD21	1.91	0.51
2:O:206:LEU:CD2	2:O:220:ALA:HB2	2.39	0.51
2:B:57:TYR:CD1	2:B:57:TYR:N	2.78	0.51
5:E:74:ILE:HG22	5:E:91:TRP:CD1	2.44	0.51
1:N:364:ALA:O	1:N:368:GLN:HG3	2.10	0.51
1:N:395:TRP:HA	1:N:395:TRP:HE3	1.73	0.51
1:N:402:VAL:HG22	1:N:406:MET:HE1	1.91	0.51
14:P:3002:UQ:HM51	14:P:3002:UQ:C8	2.41	0.51
2:B:395:PRO:HA	2:B:398:VAL:HG12	1.93	0.51
2:B:407:SER:O	2:B:411:VAL:HG23	2.11	0.51
6:F:84:GLU:CD	6:F:84:GLU:H	2.14	0.51
2:O:259:THR:CG2	2:O:260:GLU:N	2.74	0.51
4:Q:167:GLU:CG	8:U:13:LEU:HD12	2.40	0.51
3:C:101:ARG:C	3:C:101:ARG:HD2	2.30	0.51
1:N:63:ALA:O	1:N:116:VAL:HG13	2.11	0.51
5:R:134:ILE:HD12	5:R:185:TYR:HD1	1.74	0.51
8:U:22:GLU:O	8:U:26:GLN:HG2	2.10	0.51
9:V:70:LEU:HD23	9:V:71:ASN:H	1.74	0.51
2:B:47:ILE:HD11	2:B:116:VAL:HG13	1.91	0.51
3:C:153:ALA:HB2	3:C:288:LYS:HG2	1.93	0.51
2:B:76:THR:HG23	2:B:82:SER:HB2	1.92	0.51
5:E:144:CYS:HB2	5:E:158:CYS:SG	2.50	0.51
7:G:73:ASN:ND2	7:G:75:ALA:HB3	2.26	0.51
3:P:138:GLN:OE1	3:P:138:GLN:HA	2.11	0.51
8:U:40:CYS:O	8:U:44:VAL:HG23	2.11	0.51
10:W:4:ALA:O	10:W:8:GLN:HG3	2.10	0.51
1:A:187:ASP:O	1:A:191:LYS:HE3	2.10	0.51
4:D:57:THR:HB	4:D:60:GLU:HG3	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:229:VAL:CG2	7:G:20:PRO:HG3	2.40	0.51
4:Q:181:GLN:HA	8:U:77:LEU:HD22	1.91	0.51
7:T:36:ASN:O	7:T:40:ARG:HG3	2.11	0.51
17:D:2003:CDL:HB22	7:G:40:ARG:NH2	2.26	0.51
8:H:21:ARG:HG3	8:H:21:ARG:HH11	1.76	0.51
4:Q:2:GLU:O	4:Q:3:LEU:O	2.29	0.51
2:B:292:THR:O	2:B:292:THR:HG22	2.11	0.51
2:B:345:LYS:O	2:B:349:GLN:HG3	2.10	0.51
2:B:361:LYS:HA	2:B:402:ILE:HD11	1.92	0.51
17:D:2003:CDL:HA61	17:D:2003:CDL:H721	1.93	0.51
5:E:155:GLY:HA3	5:E:166:ASP:O	2.11	0.51
9:I:64:LEU:HD12	9:I:77:ARG:O	2.11	0.51
2:O:164:HIS:O	2:O:173:ALA:HA	2.11	0.51
4:Q:142:VAL:O	4:Q:142:VAL:HG23	2.11	0.51
2:O:31:ASN:HB2	2:O:201:SER:OG	2.11	0.50
2:O:57:TYR:N	2:O:57:TYR:CD1	2.79	0.50
3:P:106:GLY:HA2	3:P:108:TYR:CZ	2.46	0.50
5:R:110:ALA:HA	5:R:122:HIS:NE2	2.25	0.50
3:P:212:ILE:CD1	6:S:62:ILE:HG23	2.40	0.50
5:E:135:LEU:CD1	5:E:169:GLY:HA3	2.41	0.50
1:N:137:GLU:O	1:N:141:MET:HG3	2.10	0.50
2:O:122:TYR:O	2:O:126:VAL:HG23	2.10	0.50
3:P:350:ILE:O	3:P:354:MET:HG2	2.11	0.50
1:A:112:LEU:O	1:A:116:VAL:HG23	2.11	0.50
5:E:141:HIS:HB2	5:E:176:ALA:CB	2.40	0.50
7:T:40:ARG:HD2	17:T:3004:CDL:OA4	2.12	0.50
10:W:7:ARG:HB3	10:W:7:ARG:HH11	1.73	0.50
1:A:191:LYS:C	1:A:195:MET:HE2	2.32	0.50
4:Q:215:LEU:HD13	5:R:46:ALA:HB3	1.94	0.50
3:P:313:GLN:HE21	6:S:36:THR:CB	2.24	0.50
1:N:140:GLU:HG3	9:V:50:LEU:HD12	1.93	0.50
2:B:46:ARG:HD2	2:B:110:GLU:CD	2.32	0.50
2:B:259:THR:HG22	2:B:260:GLU:N	2.26	0.50
2:B:28:LYS:O	2:B:29:LEU:O	2.29	0.50
2:B:332:HIS:O	2:B:336:VAL:HG23	2.12	0.50
2:B:395:PRO:O	2:B:398:VAL:HG12	2.11	0.50
2:O:168:TYR:CE2	2:O:172:LEU:HD12	2.47	0.50
3:P:305:ILE:HB	3:P:306:PRO:HD3	1.93	0.50
4:Q:117:VAL:HG21	4:Q:191:ARG:HA	1.93	0.50
14:C:2002:UQ:HM51	14:C:2002:UQ:C8	2.41	0.50
12:C:502:HEM:HMC2	12:C:502:HEM:CBC	2.41	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:99:ARG:HB3	5:E:133:VAL:CG1	2.41	0.50
4:D:215:LEU:HD13	5:E:46:ALA:HB3	1.94	0.50
2:O:52:LYS:O	2:O:203:ARG:NH2	2.35	0.50
7:T:49:ALA:HB3	7:T:50:PRO:HD3	1.93	0.50
2:B:287:ARG:HB3	9:I:53:GLU:HG3	1.93	0.50
2:B:338:ARG:CG	2:B:338:ARG:NH1	2.69	0.50
5:E:189:GLY:O	5:E:192:LEU:N	2.45	0.50
8:H:28:GLU:CG	8:H:32:LYS:HE3	2.42	0.50
3:P:34:PHE:HB2	20:P:381:HOH:O	2.10	0.50
2:B:207:VAL:HG21	2:B:383:GLY:CA	2.42	0.50
2:B:59:THR:HG22	2:B:61:ALA:H	1.75	0.50
3:C:328:LEU:HD12	7:G:51:PRO:CB	2.32	0.50
3:C:78:TRP:CZ3	4:D:201:ARG:HG3	2.47	0.50
3:C:313:GLN:HE21	6:F:36:THR:CB	2.25	0.50
1:N:279:ARG:HH22	9:V:30:UNK:C	2.23	0.50
1:N:281:ASP:O	1:N:283:THR:N	2.45	0.50
2:O:56:ARG:NH1	2:O:172:LEU:HG	2.27	0.50
5:R:131:GLU:N	5:R:131:GLU:OE1	2.45	0.50
1:A:307:PHE:C	1:A:307:PHE:CD1	2.85	0.50
2:B:52:LYS:O	2:B:203:ARG:NH2	2.41	0.50
3:C:41:CYS:SG	3:C:90:PHE:HD2	2.35	0.50
5:E:190:ASP:O	5:E:192:LEU:N	2.44	0.50
1:N:280:TYR:CG	1:N:281:ASP:N	2.79	0.50
3:P:156:TYR:C	3:P:158:GLY:H	2.13	0.50
3:C:286:PRO:O	3:C:287:ASN:HB2	2.12	0.49
4:D:102:ARG:HB3	4:D:107:GLY:HA2	1.94	0.49
4:D:169:LEU:HD23	4:D:169:LEU:C	2.32	0.49
5:E:130:PRO:HG2	5:E:131:GLU:OE2	2.11	0.49
5:E:82:PRO:HG2	5:E:85:LYS:HB2	1.94	0.49
2:O:345:LYS:O	2:O:349:GLN:HG3	2.12	0.49
2:O:361:LYS:HD3	2:O:403:ASP:HA	1.94	0.49
5:R:165:TYR:HA	5:R:170:ARG:O	2.12	0.49
5:E:165:TYR:HA	5:E:170:ARG:O	2.12	0.49
1:N:7:THR:HG21	2:O:113:ARG:CD	2.39	0.49
2:O:286:LYS:HE2	2:O:287:ARG:HH12	1.77	0.49
1:A:137:GLU:O	1:A:141:MET:HG3	2.12	0.49
1:A:158:PHE:O	1:A:164:ALA:HB2	2.12	0.49
1:A:85:HIS:HB2	1:A:100:LYS:HB2	1.93	0.49
2:B:56:ARG:NH1	2:B:172:LEU:HG	2.26	0.49
1:N:382:HIS:HB3	1:N:388:ARG:O	2.12	0.49
5:R:144:CYS:HB2	5:R:158:CYS:SG	2.51	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:97:PHE:O	5:R:134:ILE:HA	2.13	0.49
6:S:77:LYS:HA	6:S:80:TRP:CE2	2.48	0.49
3:C:90:PHE:CE1	3:C:236:MET:HB3	2.48	0.49
5:E:106:ILE:O	5:E:106:ILE:HG22	2.11	0.49
2:B:314:VAL:CG1	9:I:63:ASP:HB3	2.40	0.49
2:O:212:LYS:HB3	2:O:215:ASP:OD2	2.12	0.49
3:P:325:LEU:HD21	3:P:366:LEU:HB3	1.93	0.49
8:U:21:ARG:HG3	8:U:21:ARG:NH1	2.27	0.49
1:A:173:ASN:O	1:A:177:LEU:HG	2.12	0.49
1:A:371:GLY:O	1:A:375:VAL:HG23	2.12	0.49
1:A:49:ASN:ND2	1:A:51:LYS:H	2.10	0.49
4:D:169:LEU:HD23	4:D:169:LEU:O	2.11	0.49
3:P:334:LEU:HD21	11:P:3007:PEE:H65	1.93	0.49
4:Q:79:GLU:HA	4:Q:79:GLU:OE2	2.13	0.49
1:A:220:SER:HB2	1:A:225:GLU:HB2	1.95	0.49
3:C:263:LEU:O	3:C:264:VAL:CG2	2.61	0.49
1:N:10:ASN:ND2	2:O:19:PRO:CD	2.71	0.49
3:P:263:LEU:O	3:P:264:VAL:CG2	2.61	0.49
3:P:286:PRO:O	3:P:287:ASN:HB2	2.13	0.49
2:B:109:VAL:HG21	2:B:119:VAL:HG12	1.95	0.49
5:E:97:PHE:O	5:E:134:ILE:HA	2.12	0.49
5:E:188:VAL:HG12	5:E:188:VAL:O	2.12	0.49
1:N:10:ASN:CG	2:O:19:PRO:HD2	2.33	0.49
2:O:357:VAL:CG1	2:O:361:LYS:HE3	2.43	0.49
3:P:198:LEU:HD21	12:P:502:HEM:HMA3	1.93	0.49
4:Q:47:ALA:HA	4:Q:90:TYR:HA	1.95	0.49
5:R:177:PRO:HG2	5:R:178:TYR:H	1.77	0.49
3:C:305:ILE:HB	3:C:306:PRO:HD3	1.95	0.49
4:Q:102:ARG:HB3	4:Q:107:GLY:HA2	1.95	0.49
5:R:118:ARG:NH1	5:R:174:GLY:O	2.45	0.49
10:W:40:ASP:O	10:W:44:GLU:HG3	2.11	0.49
10:W:58:LYS:HB2	10:W:59:TYR:CE1	2.48	0.49
3:C:50:LEU:O	3:C:54:MET:HG3	2.12	0.49
4:Q:171:TYR:OH	4:Q:182:ILE:HA	2.13	0.49
2:B:27:THR:CG2	2:B:28:LYS:N	2.74	0.49
4:D:165:TYR:CZ	4:D:168:ILE:HG13	2.48	0.49
2:O:292:THR:HG22	2:O:292:THR:O	2.13	0.49
2:B:164:HIS:O	2:B:173:ALA:HA	2.13	0.48
2:B:353:THR:HG22	2:B:355:GLU:N	2.03	0.48
1:N:220:SER:HB2	1:N:225:GLU:HB2	1.94	0.48
1:N:60:GLU:OE2	1:N:89:TYR:HA	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:59:THR:HG22	2:O:60:THR:N	2.27	0.48
1:A:64:PHE:HE2	1:A:86:PHE:CE1	2.31	0.48
4:D:70:VAL:HG21	4:D:83:ARG:CZ	2.43	0.48
2:O:133:ARG:HD3	2:O:135:TRP:CZ2	2.47	0.48
4:Q:1:GLY:O	4:Q:2:GLU:HB2	2.13	0.48
4:D:171:TYR:OH	4:D:182:ILE:HA	2.13	0.48
5:E:73:LYS:HB3	5:E:196:GLY:O	2.12	0.48
7:G:34:LEU:HB2	7:G:35:PRO:HD3	1.94	0.48
2:O:395:PRO:HA	2:O:398:VAL:HG12	1.95	0.48
2:O:402:ILE:HG23	2:O:403:ASP:N	2.28	0.48
5:R:129:LYS:HB3	5:R:131:GLU:OE1	2.13	0.48
4:Q:237:TYR:HB2	6:S:60:PHE:CD1	2.48	0.48
8:U:17:LEU:HD13	8:U:73:LEU:HD22	1.96	0.48
8:U:43:ARG:HD2	8:U:47:ARG:NH2	2.28	0.48
2:B:324:PHE:HE2	2:B:341:MET:HE3	1.79	0.48
4:D:181:GLN:HA	8:H:77:LEU:HD22	1.93	0.48
4:D:57:THR:CG2	4:D:58:GLU:N	2.75	0.48
6:F:58:ARG:HD2	6:F:89:TYR:OH	2.13	0.48
8:H:17:LEU:HD13	8:H:73:LEU:HD22	1.94	0.48
9:I:34:UNK:CG	9:I:35:UNK:N	2.76	0.48
1:N:219:VAL:HG12	1:N:220:SER:N	2.27	0.48
1:N:64:PHE:HE2	1:N:86:PHE:CE1	2.32	0.48
3:P:263:LEU:O	3:P:264:VAL:HG23	2.13	0.48
5:R:155:GLY:HA3	5:R:166:ASP:O	2.13	0.48
5:R:186:GLN:O	5:R:193:VAL:HG23	2.14	0.48
5:R:78:LEU:HD11	5:R:187:PHE:HD1	1.77	0.48
6:S:84:GLU:H	6:S:84:GLU:CD	2.16	0.48
1:A:27:SER:HA	1:A:199:ALA:O	2.13	0.48
2:B:168:TYR:CE2	2:B:172:LEU:HD12	2.48	0.48
2:B:353:THR:HG22	2:B:354:GLU:N	2.28	0.48
5:E:178:TYR:CD1	5:E:178:TYR:N	2.82	0.48
3:P:325:LEU:HD22	3:P:370:ILE:HG13	1.96	0.48
5:R:170:ARG:HA	5:R:179:ASN:CB	2.39	0.48
3:C:45:GLN:HB3	12:C:501:HEM:HAB	1.94	0.48
2:O:170:THR:O	2:O:172:LEU:N	2.47	0.48
2:O:31:ASN:ND2	2:O:31:ASN:N	2.58	0.48
5:R:119:ASP:HB3	5:R:179:ASN:HD21	1.77	0.48
2:B:264:VAL:HG23	2:B:316:TYR:O	2.13	0.48
2:B:56:ARG:HH11	2:B:56:ARG:HG3	1.79	0.48
5:E:189:GLY:O	5:E:192:LEU:O	2.32	0.48
5:E:83:GLU:C	5:E:85:LYS:H	2.16	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:134:ILE:CG2	1:N:174:ILE:HD13	2.43	0.48
1:N:85:HIS:HB2	1:N:100:LYS:HB2	1.95	0.48
3:P:279:TYR:O	3:P:282:LEU:HB3	2.14	0.48
2:B:110:GLU:O	2:B:111:CYS:HB3	2.14	0.48
2:B:259:THR:CG2	2:B:260:GLU:N	2.77	0.48
9:I:31:UNK:CA	9:I:73:PRO:HG2	2.44	0.48
1:N:321:GLY:HA2	1:N:342:TRP:HZ2	1.79	0.48
3:P:28:ILE:HD11	3:P:225:TYR:CE2	2.48	0.48
1:A:223:TYR:HD2	1:A:223:TYR:H	1.60	0.48
1:A:364:ALA:O	1:A:368:GLN:HG3	2.14	0.48
7:G:50:PRO:HB2	7:G:51:PRO:HD3	1.96	0.48
3:P:30:ALA:HB1	17:Q:3003:CDL:H111	1.95	0.48
5:R:162:GLY:O	5:R:163:SER:C	2.51	0.48
7:T:34:LEU:HB2	7:T:35:PRO:HD3	1.96	0.48
7:T:65:GLU:O	7:T:69:LEU:HG	2.13	0.48
1:A:248:LEU:HD12	1:A:426:GLY:HA2	1.94	0.48
5:E:77:LYS:HA	5:E:192:LEU:HD23	1.96	0.48
1:N:45:SER:HA	1:N:48:GLU:HG3	1.95	0.48
5:R:135:LEU:HD13	5:R:180:LEU:HD12	1.95	0.48
1:A:358:LYS:HE3	1:A:399:ILE:O	2.14	0.47
1:A:395:TRP:HA	1:A:395:TRP:HE3	1.78	0.47
5:E:190:ASP:C	5:E:192:LEU:N	2.67	0.47
10:J:40:ASP:O	10:J:44:GLU:HG3	2.14	0.47
8:U:65:ARG:O	8:U:68:CYS:HB3	2.14	0.47
2:O:71:LEU:CD2	9:V:68:ILE:HG13	2.44	0.47
4:Q:195:GLU:OE1	4:Q:201:ARG:NH2	2.47	0.47
5:R:77:LYS:HE2	5:R:79:SER:HB2	1.95	0.47
6:F:77:LYS:HE2	6:F:77:LYS:HB3	1.74	0.47
1:N:106:MET:HG3	1:N:203:ILE:CD1	2.37	0.47
1:N:358:LYS:HE3	1:N:399:ILE:O	2.14	0.47
5:R:178:TYR:N	5:R:178:TYR:HD1	2.12	0.47
6:S:95:LYS:O	6:S:99:ARG:HG3	2.14	0.47
1:A:320:PHE:CE2	1:A:415:ILE:HD11	2.50	0.47
2:B:28:LYS:HG2	2:B:28:LYS:O	2.14	0.47
3:C:121:LEU:O	3:C:125:MET:HG3	2.14	0.47
5:E:75:GLU:HB3	5:E:194:VAL:HG22	1.95	0.47
6:F:77:LYS:HA	6:F:80:TRP:CE2	2.49	0.47
1:N:151:ASP:OD2	5:R:2:HIS:NE2	2.31	0.47
1:N:191:LYS:CA	1:N:195:MET:HE2	2.44	0.47
2:O:227:ARG:HB3	2:O:228:SER:H	1.52	0.47
2:O:414:ALA:O	2:O:418:VAL:HG23	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:56:ARG:HG3	2:O:56:ARG:NH1	2.28	0.47
3:P:92:PHE:O	3:P:95:ILE:HG22	2.14	0.47
4:Q:240:PRO:O	4:Q:241:LYS:C	2.53	0.47
5:R:49:TYR:HE1	10:W:32:GLU:HG3	1.79	0.47
2:B:47:ILE:CD1	2:B:120:MET:HE2	2.42	0.47
2:B:215:ASP:O	2:B:219:VAL:HG23	2.15	0.47
5:E:142:LEU:HD12	5:E:161:HIS:CE1	2.49	0.47
9:I:49:LEU:HD22	9:I:54:SER:HB3	1.96	0.47
2:O:29:LEU:HB2	2:O:31:ASN:HD21	1.79	0.47
1:A:151:ASP:OD2	5:E:2:HIS:NE2	2.33	0.47
3:C:92:PHE:O	3:C:95:ILE:HG22	2.13	0.47
1:N:288:LYS:HE3	1:N:289:HIS:CE1	2.49	0.47
1:N:320:PHE:CE2	1:N:415:ILE:HD11	2.49	0.47
1:N:248:LEU:HD12	1:N:426:GLY:HA2	1.97	0.47
4:Q:102:ARG:HA	4:Q:108:ALA:O	2.14	0.47
10:W:7:ARG:NH1	10:W:7:ARG:CB	2.75	0.47
5:R:185:TYR:HB3	5:R:195:VAL:HA	1.96	0.47
1:A:217:SER:O	1:A:218:GLY:C	2.53	0.47
4:D:134:TYR:CG	4:D:162:PRO:HG3	2.50	0.47
5:E:127:VAL:O	5:E:128:LYS:HB2	2.15	0.47
2:O:303:THR:HA	2:O:335:GLU:OE1	2.15	0.47
2:O:325:TYR:CD1	9:V:60:ALA:HB3	2.50	0.47
2:O:76:THR:HG23	2:O:82:SER:HB2	1.97	0.47
4:Q:149:TYR:CE1	4:Q:156:GLN:HB3	2.50	0.47
5:R:113:ASP:HB2	5:R:116:LYS:HB2	1.96	0.47
5:R:185:TYR:O	5:R:186:GLN:HB3	2.14	0.47
5:R:75:GLU:O	5:R:75:GLU:HG3	2.15	0.47
2:B:76:THR:HG23	2:B:136:GLU:OE1	2.15	0.47
2:B:402:ILE:HG23	2:B:403:ASP:N	2.30	0.47
1:N:281:ASP:HB2	9:V:33:UNK:HB2	1.95	0.47
2:O:385:GLU:O	2:O:389:SER:HB3	2.14	0.47
4:Q:240:PRO:HD3	7:T:12:HIS:CE1	2.50	0.47
2:B:306:PRO:HA	9:I:52:ARG:HG3	1.95	0.47
2:B:357:VAL:CG1	2:B:361:LYS:HE3	2.45	0.47
4:D:208:MET:O	4:D:212:SER:HB2	2.15	0.47
4:D:69:GLU:OE1	4:D:82:MET:HB3	2.15	0.47
3:P:108:TYR:HB3	3:P:114:TRP:CE3	2.50	0.47
8:U:34:ARG:O	8:U:38:GLU:HG3	2.15	0.47
1:A:70:ARG:HA	1:A:71:PRO:HD2	1.80	0.47
3:C:224:TYR:HB3	4:D:227:TRP:CZ2	2.50	0.47
5:E:122:HIS:HB3	5:E:125:ASP:OD1	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:235:MET:CB	7:G:15:THR:HG22	2.45	0.47
1:N:205:HIS:O	1:N:208:LEU:HB3	2.15	0.47
3:P:50:LEU:O	3:P:54:MET:HG3	2.15	0.47
5:R:135:LEU:CD2	5:R:182:VAL:HG22	2.42	0.47
5:R:84:GLY:O	5:R:85:LYS:HD3	2.14	0.47
1:A:204:SER:HB3	1:A:207:GLU:HB2	1.97	0.46
7:G:36:ASN:O	7:G:40:ARG:HG3	2.15	0.46
2:O:47:ILE:CD1	2:O:116:VAL:HG13	2.44	0.46
3:P:156:TYR:CD2	3:P:156:TYR:N	2.80	0.46
3:P:238:THR:HB	3:P:239:PRO:CD	2.40	0.46
2:B:47:ILE:CD1	2:B:116:VAL:HG13	2.46	0.46
4:D:57:THR:HG22	4:D:58:GLU:N	2.29	0.46
5:E:75:GLU:O	5:E:75:GLU:HG3	2.15	0.46
8:H:43:ARG:O	8:H:47:ARG:HG3	2.15	0.46
2:O:332:HIS:O	2:O:336:VAL:HG23	2.15	0.46
4:Q:68:VAL:HG11	4:Q:92:PRO:HG3	1.97	0.46
2:B:101:THR:OG1	2:B:104:LYS:HG3	2.15	0.46
3:P:22:LEU:HD21	14:P:3002:UQ:CM3	2.45	0.46
7:T:80:ASP:OD1	8:U:47:ARG:HD3	2.15	0.46
2:O:156:GLN:NE2	9:V:77:ARG:C	2.68	0.46
2:B:402:ILE:O	2:B:405:VAL:HG23	2.16	0.46
4:D:203:ARG:NH1	18:D:2091:BOG:O3	2.49	0.46
1:N:245:ASP:OD1	7:T:11:ARG:NE	2.44	0.46
10:W:32:GLU:HG2	10:W:36:ASP:OD2	2.15	0.46
2:B:24:LEU:O	2:B:24:LEU:HG	2.16	0.46
5:E:187:PHE:C	5:E:189:GLY:N	2.68	0.46
5:E:191:ASP:N	5:E:191:ASP:OD2	2.48	0.46
9:I:71:ASN:HD22	9:I:71:ASN:H	1.64	0.46
1:N:307:PHE:CD1	1:N:307:PHE:C	2.88	0.46
3:P:90:PHE:CE1	3:P:236:MET:HB3	2.51	0.46
4:Q:158:ILE:HG12	4:Q:160:MET:H	1.81	0.46
2:B:411:VAL:O	2:B:415:LYS:HG3	2.15	0.46
2:B:414:ALA:O	2:B:418:VAL:HG23	2.15	0.46
1:N:158:PHE:O	1:N:164:ALA:HB2	2.15	0.46
4:Q:3:LEU:N	4:Q:3:LEU:HD12	2.31	0.46
4:Q:69:GLU:OE1	4:Q:82:MET:HB3	2.16	0.46
3:P:328:LEU:CD1	7:T:51:PRO:HB3	2.35	0.46
1:N:282:ARG:NH2	9:V:36:UNK:HA	2.24	0.46
9:V:51:CYS:HB2	9:V:53:GLU:OE1	2.16	0.46
2:B:385:GLU:O	2:B:387:LEU:N	2.49	0.46
4:D:117:VAL:HG21	4:D:191:ARG:HA	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:91:TRP:HZ2	5:E:196:GLY:HA2	1.80	0.46
9:V:70:LEU:CD2	9:V:71:ASN:OD1	2.64	0.46
2:B:225:ASN:O	2:B:226:ILE:C	2.53	0.46
2:B:274:VAL:O	2:B:278:VAL:HG23	2.15	0.46
3:C:279:TYR:O	3:C:282:LEU:HB3	2.16	0.46
1:N:27:SER:HA	1:N:199:ALA:O	2.16	0.46
2:O:110:GLU:O	2:O:111:CYS:HB3	2.15	0.46
4:Q:139:ALA:HB2	8:U:41:ASP:OD1	2.16	0.46
1:N:22:GLY:O	1:N:193:PRO:HA	2.15	0.46
3:P:153:ALA:CB	3:P:288:LYS:HG2	2.45	0.46
4:Q:57:THR:HB	4:Q:60:GLU:HG3	1.98	0.46
5:R:106:ILE:HG21	5:R:130:PRO:HB3	1.97	0.46
1:A:26:ALA:O	1:A:198:ALA:HA	2.16	0.46
1:A:239:SER:HB2	7:G:17:SER:O	2.16	0.46
3:C:138:GLN:HB2	3:C:255:GLU:O	2.16	0.46
5:E:141:HIS:HB3	19:E:501:FES:S2	2.55	0.46
4:Q:8:PRO:HG2	4:Q:10:PHE:CE1	2.51	0.46
5:R:137:GLY:O	5:R:145:VAL:HG13	2.15	0.46
5:R:76:ILE:O	5:R:193:VAL:HG12	2.16	0.46
5:E:41:ALA:O	5:E:45:VAL:HG23	2.16	0.45
1:N:383:LEU:O	1:N:387:GLY:HA2	2.16	0.45
2:O:46:ARG:HD2	2:O:110:GLU:CD	2.36	0.45
2:O:109:VAL:HG21	2:O:119:VAL:HG12	1.98	0.45
2:O:353:THR:HG22	2:O:354:GLU:N	2.31	0.45
4:Q:221:TYR:CD2	5:R:39:VAL:HG11	2.51	0.45
5:R:106:ILE:O	5:R:109:GLU:HB3	2.15	0.45
6:S:16:ILE:O	6:S:19:TRP:HB3	2.16	0.45
6:S:52:GLU:OE2	7:T:11:ARG:NH1	2.49	0.45
1:A:49:ASN:HD21	1:A:51:LYS:CE	2.28	0.45
5:R:140:THR:OG1	5:R:176:ALA:HB1	2.16	0.45
5:R:96:LEU:HD12	5:R:135:LEU:O	2.16	0.45
1:A:233:ARG:HH21	1:A:316:ASP:HB2	1.81	0.45
1:A:402:VAL:HA	1:A:406:MET:CE	2.46	0.45
2:B:104:LYS:C	2:B:104:LYS:HD2	2.37	0.45
4:D:102:ARG:NH1	4:D:102:ARG:HG2	2.31	0.45
6:F:13:MET:O	6:F:17:ARG:HG3	2.16	0.45
2:B:71:LEU:CD2	9:I:68:ILE:HG13	2.47	0.45
2:B:156:GLN:HE22	9:I:77:ARG:C	2.20	0.45
1:N:223:TYR:HD2	1:N:223:TYR:H	1.64	0.45
4:Q:57:THR:CG2	4:Q:58:GLU:N	2.79	0.45
5:R:171:ILE:HD13	5:R:176:ALA:HB3	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:188:VAL:O	5:R:192:LEU:HB2	2.16	0.45
10:W:59:TYR:N	10:W:59:TYR:CD1	2.84	0.45
5:E:76:ILE:O	5:E:193:VAL:HG12	2.17	0.45
1:N:106:MET:HE2	1:N:106:MET:O	2.17	0.45
1:N:122:LEU:HD11	1:N:186:ILE:HD12	1.99	0.45
1:N:240:GLU:HA	1:N:422:LEU:O	2.17	0.45
4:Q:102:ARG:HG2	4:Q:102:ARG:HH11	1.80	0.45
5:R:184:THR:O	5:R:185:TYR:HB3	2.16	0.45
5:R:77:LYS:HA	5:R:192:LEU:HD23	1.97	0.45
1:A:144:ASP:OD2	1:A:147:ASN:ND2	2.49	0.45
1:A:178:THR:HG22	1:A:179:ARG:N	2.31	0.45
11:C:2007:PEE:H11	6:F:29:TYR:OH	2.16	0.45
7:G:81:GLN:HG3	7:G:81:GLN:OXT	2.17	0.45
2:O:169:LYS:O	2:O:170:THR:HG23	2.15	0.45
2:O:247:GLN:HE22	2:O:429:ASP:HA	1.82	0.45
3:P:18:SER:CB	3:P:202:HIS:HE1	2.30	0.45
1:A:382:HIS:HB3	1:A:388:ARG:O	2.17	0.45
2:B:86:THR:O	2:B:90:GLU:HG3	2.17	0.45
2:B:325:TYR:CD1	9:I:60:ALA:HB3	2.52	0.45
11:P:3007:PEE:H7	7:T:44:GLN:HE21	1.81	0.45
4:Q:168:ILE:HG12	4:Q:168:ILE:O	2.16	0.45
2:O:307:PHE:H	9:V:52:ARG:HG2	1.82	0.45
2:B:303:THR:HA	2:B:335:GLU:OE1	2.17	0.45
5:E:84:GLY:N	5:E:100:HIS:O	2.44	0.45
6:F:67:ASP:HA	6:F:70:LEU:HD23	1.99	0.45
7:G:28:ASN:HB3	7:G:31:SER:OG	2.17	0.45
1:N:26:ALA:O	1:N:198:ALA:HA	2.17	0.45
1:N:49:ASN:HD21	1:N:51:LYS:CE	2.30	0.45
2:O:345:LYS:HG2	2:O:418:VAL:CG1	2.46	0.45
3:P:208:ASN:HB2	3:P:209:PRO:HD2	1.99	0.45
5:R:112:VAL:HG21	5:R:170:ARG:NH2	2.32	0.45
1:N:143:ASN:ND2	9:V:48:PRO:HD3	2.25	0.45
1:A:134:ILE:CG2	1:A:174:ILE:HD13	2.47	0.45
2:B:72:ALA:HB1	2:B:75:LEU:HD12	1.97	0.45
6:F:40:ASP:O	6:F:44:LYS:HG3	2.17	0.45
2:O:35:ILE:HD13	2:O:217:LYS:HA	1.99	0.45
2:O:286:LYS:C	2:O:288:GLY:H	2.20	0.45
2:O:345:LYS:HG2	2:O:418:VAL:HG13	1.99	0.45
2:O:46:ARG:HD2	2:O:110:GLU:HG2	1.99	0.45
2:O:54:GLY:C	2:O:56:ARG:H	2.20	0.45
2:O:86:THR:O	2:O:90:GLU:HG3	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:26:VAL:HG22	4:Q:188:THR:HG22	1.98	0.45
1:A:222:THR:OG1	1:A:225:GLU:HG3	2.17	0.45
5:E:137:GLY:O	5:E:145:VAL:HG13	2.16	0.45
4:Q:200:GLN:NE2	18:Q:3091:BOG:H5	2.32	0.45
1:N:106:MET:HE2	1:N:110:VAL:CG2	2.47	0.45
1:N:23:LEU:HD23	1:N:24:ARG:N	2.31	0.45
3:P:376:LYS:O	6:S:17:ARG:NH1	2.47	0.45
2:B:71:LEU:CD1	2:B:144:LEU:HD23	2.46	0.44
3:C:234:THR:HG21	4:D:219:LEU:HD12	1.99	0.44
5:E:73:LYS:HB2	5:E:195:VAL:O	2.16	0.44
1:N:191:LYS:C	1:N:195:MET:HE2	2.37	0.44
5:R:163:SER:HA	5:R:174:GLY:HA3	1.99	0.44
2:B:247:GLN:HE22	2:B:429:ASP:HA	1.83	0.44
4:D:222:MET:HE3	5:E:40:THR:HG23	1.99	0.44
6:F:13:MET:HA	6:F:13:MET:HE2	1.98	0.44
10:J:32:GLU:HG2	10:J:36:ASP:OD2	2.17	0.44
5:R:161:HIS:CB	5:R:175:PRO:HG3	2.47	0.44
5:R:169:GLY:O	5:R:179:ASN:HB3	2.17	0.44
1:A:205:HIS:O	1:A:208:LEU:HB3	2.18	0.44
1:A:274:ASN:HD22	1:A:274:ASN:HA	1.65	0.44
5:E:127:VAL:CG1	5:E:128:LYS:H	2.13	0.44
9:I:68:ILE:HD13	9:I:68:ILE:HA	1.85	0.44
2:O:75:LEU:HD22	2:O:136:GLU:HB3	1.99	0.44
10:J:56:LYS:HE2	10:J:56:LYS:HB3	1.82	0.44
4:Q:161:ALA:O	4:Q:162:PRO:C	2.56	0.44
5:R:179:ASN:O	5:R:180:LEU:C	2.56	0.44
1:A:35:CYS:SG	1:A:203:ILE:HD11	2.57	0.44
2:B:402:ILE:HG23	2:B:403:ASP:H	1.83	0.44
5:E:136:VAL:O	5:E:138:VAL:N	2.44	0.44
2:O:26:ILE:O	2:O:26:ILE:HG12	2.16	0.44
4:Q:57:THR:HG22	4:Q:58:GLU:N	2.32	0.44
5:R:171:ILE:HG12	5:R:176:ALA:O	2.18	0.44
2:B:295:LEU:O	2:B:299:VAL:HG23	2.18	0.44
11:C:2007:PEE:H7	7:G:44:GLN:HE21	1.81	0.44
4:D:168:ILE:HG12	4:D:168:ILE:O	2.18	0.44
17:Q:3003:CDL:H721	17:Q:3003:CDL:HA61	1.99	0.44
9:V:64:LEU:HD12	9:V:77:ARG:C	2.36	0.44
2:B:170:THR:O	2:B:172:LEU:N	2.50	0.44
3:C:286:PRO:O	3:C:287:ASN:CB	2.65	0.44
16:D:501:HEC:HBB3	16:D:501:HEC:HMB1	2.00	0.44
1:N:438:ARG:HH11	1:N:438:ARG:HG3	1.83	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:275:PHE:HB3	13:P:3001:AZO:C11	2.48	0.44
1:N:402:VAL:HA	1:N:406:MET:CE	2.48	0.44
2:O:162:ASN:O	2:O:244:ILE:HD12	2.18	0.44
2:O:221:GLU:CG	2:O:222:GLN:H	2.25	0.44
2:O:411:VAL:O	2:O:415:LYS:HG3	2.18	0.44
3:P:18:SER:HB2	3:P:202:HIS:HE1	1.82	0.44
3:P:28:ILE:HD11	3:P:225:TYR:CZ	2.53	0.44
5:R:165:TYR:CD2	5:R:180:LEU:HG	2.53	0.44
9:V:33:UNK:HA	9:V:73:PRO:HB3	2.00	0.44
2:B:333:ALA:O	2:B:337:ILE:HG13	2.18	0.44
3:C:49:GLY:O	12:C:501:HEM:HAC	2.17	0.44
1:A:26:ALA:HB2	1:A:383:LEU:HD11	1.99	0.43
2:B:56:ARG:NH1	2:B:56:ARG:HG3	2.33	0.43
3:C:106:GLY:HA2	3:C:108:TYR:CZ	2.53	0.43
5:E:114:VAL:HG21	5:E:172:ARG:HH12	1.83	0.43
5:E:133:VAL:HG13	5:E:133:VAL:O	2.18	0.43
5:E:96:LEU:HD12	5:E:135:LEU:O	2.18	0.43
5:E:129:LYS:HG3	5:E:187:PHE:CE2	2.53	0.43
8:H:34:ARG:O	8:H:38:GLU:HG3	2.18	0.43
5:E:49:TYR:CE1	10:J:32:GLU:HG3	2.53	0.43
10:J:58:LYS:HB2	10:J:59:TYR:CE1	2.53	0.43
2:O:207:VAL:HG21	2:O:383:GLY:CA	2.46	0.43
3:P:27:ASN:ND2	3:P:209:PRO:HG2	2.32	0.43
3:P:41:CYS:SG	3:P:91:PHE:HA	2.58	0.43
4:Q:2:GLU:HB3	4:Q:3:LEU:HD12	2.00	0.43
6:S:58:ARG:HD2	6:S:89:TYR:OH	2.18	0.43
1:A:217:SER:O	1:A:219:VAL:HG23	2.18	0.43
1:N:239:SER:HB2	7:T:17:SER:O	2.18	0.43
5:R:103:GLN:O	5:R:107:ASN:ND2	2.51	0.43
1:A:205:HIS:O	1:A:209:VAL:HG12	2.18	0.43
2:B:132:PHE:CE1	2:B:191:LEU:HB3	2.53	0.43
3:C:153:ALA:CB	3:C:288:LYS:HG2	2.49	0.43
4:D:105:ASN:O	4:D:106:ASN:HB2	2.18	0.43
3:P:286:PRO:O	3:P:287:ASN:CB	2.66	0.43
2:B:220:ALA:O	2:B:224:LEU:HB2	2.18	0.43
2:B:68:LEU:HD23	2:B:186:ILE:HG21	2.00	0.43
4:D:234:LYS:HD2	5:E:8:PRO:HB2	2.00	0.43
1:N:134:ILE:HG22	1:N:174:ILE:HD13	2.00	0.43
2:O:324:PHE:HE2	2:O:341:MET:HE3	1.83	0.43
3:P:101:ARG:O	3:P:101:ARG:HD2	2.18	0.43
3:P:263:LEU:C	3:P:264:VAL:HG23	2.39	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:GLY:HA2	1:A:342:TRP:HZ2	1.83	0.43
2:B:33:LEU:HD12	2:B:204:MET:O	2.19	0.43
2:B:46:ARG:HD2	2:B:110:GLU:HG2	2.00	0.43
4:D:223:LYS:HD3	4:D:223:LYS:C	2.38	0.43
1:N:362:ARG:O	1:N:365:MET:HG2	2.18	0.43
2:O:33:LEU:HD12	2:O:204:MET:O	2.17	0.43
4:Q:238:ARG:CZ	5:R:5:VAL:HG22	2.48	0.43
2:B:168:TYR:HB2	2:B:173:ALA:HB2	2.00	0.43
2:B:54:GLY:C	2:B:56:ARG:H	2.21	0.43
1:N:17:THR:HG23	1:N:205:HIS:NE2	2.34	0.43
5:R:101:ARG:HH21	5:R:130:PRO:HA	1.83	0.43
1:A:274:ASN:ND2	1:A:309:THR:HB	2.34	0.43
3:C:120:LEU:HD23	3:C:120:LEU:HA	1.87	0.43
3:C:273:TRP:HA	3:C:276:LEU:CD1	2.48	0.43
11:C:2007:PEE:H50	17:G:2004:CDL:H712	2.01	0.43
2:O:222:GLN:HG2	2:O:222:GLN:O	2.19	0.43
3:P:198:LEU:HD13	14:P:3002:UQ:HM53	2.01	0.43
5:R:96:LEU:HD21	5:R:195:VAL:HG21	2.00	0.43
5:R:79:SER:OG	5:R:191:ASP:HB2	2.18	0.43
1:A:331:ILE:CG2	1:A:431:LEU:HB2	2.41	0.43
5:E:162:GLY:O	5:E:163:SER:C	2.57	0.43
1:N:178:THR:HG22	1:N:179:ARG:N	2.33	0.43
1:N:354:VAL:HG23	1:N:355:LYS:N	2.34	0.43
9:I:39:UNK:HA	9:V:40:UNK:O	2.19	0.43
1:A:21:ASN:N	1:A:21:ASN:OD1	2.49	0.43
2:B:297:GLN:O	2:B:301:LYS:HG3	2.18	0.43
8:H:21:ARG:HG3	8:H:21:ARG:NH1	2.34	0.43
2:O:141:GLN:N	2:O:142:PRO:HD2	2.34	0.43
7:T:28:ASN:HB3	7:T:31:SER:OG	2.19	0.43
1:A:106:MET:C	1:A:106:MET:HE2	2.39	0.43
1:A:40:TRP:CZ2	1:A:377:GLU:HA	2.54	0.43
1:A:418:LYS:O	1:A:420:PRO:HD3	2.19	0.43
1:A:438:ARG:HH11	1:A:438:ARG:HG3	1.84	0.43
2:O:71:LEU:CD1	2:O:144:LEU:HD23	2.48	0.43
2:O:395:PRO:O	2:O:398:VAL:HG12	2.18	0.43
5:R:133:VAL:HG13	5:R:133:VAL:O	2.19	0.43
4:Q:235:MET:CB	7:T:15:THR:HG22	2.45	0.43
8:U:21:ARG:HD2	8:U:65:ARG:NH1	2.33	0.43
2:B:209:ILE:HG22	2:B:210:GLY:N	2.34	0.42
2:B:35:ILE:HD13	2:B:217:LYS:HA	2.01	0.42
2:B:395:PRO:O	2:B:398:VAL:CG1	2.67	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:239:PRO:C	4:D:241:LYS:H	2.20	0.42
5:E:164:HIS:HD2	5:E:173:LYS:HB3	1.84	0.42
1:N:106:MET:N	1:N:107:PRO:HD2	2.34	0.42
2:O:402:ILE:HG23	2:O:403:ASP:H	1.84	0.42
5:R:184:THR:HG22	5:R:185:TYR:N	2.34	0.42
2:B:399:ALA:O	2:B:402:ILE:CG2	2.63	0.42
5:E:130:PRO:C	5:E:132:TRP:H	2.21	0.42
6:F:16:ILE:O	6:F:19:TRP:HB3	2.19	0.42
1:N:170:THR:HG22	1:N:171:THR:H	1.84	0.42
1:N:189:HIS:ND1	1:N:194:ARG:NH2	2.62	0.42
2:O:18:CYS:CB	2:O:19:PRO:CD	2.97	0.42
5:E:151:GLY:O	5:E:154:GLY:N	2.52	0.42
5:E:164:HIS:CD2	5:E:173:LYS:HB3	2.53	0.42
5:E:171:ILE:HG23	5:E:171:ILE:O	2.18	0.42
5:E:77:LYS:HG3	5:E:191:ASP:O	2.18	0.42
2:O:264:VAL:HG12	2:O:265:GLY:N	2.34	0.42
8:U:65:ARG:O	8:U:69:VAL:HG23	2.20	0.42
14:C:2002:UQ:HM51	14:C:2002:UQ:H8	2.01	0.42
17:D:2003:CDL:OB3	6:F:73:ARG:NH2	2.52	0.42
1:N:271:HIS:CE1	1:N:311:ASN:HD22	2.37	0.42
3:P:9:HIS:CD2	3:P:11:LEU:HB2	2.54	0.42
4:Q:105:ASN:O	4:Q:106:ASN:HB2	2.19	0.42
5:R:100:HIS:HD2	5:R:131:GLU:O	2.02	0.42
6:S:98:ILE:O	6:S:102:LEU:HG	2.20	0.42
1:A:191:LYS:N	1:A:195:MET:HE2	2.35	0.42
2:B:353:THR:CG2	2:B:354:GLU:N	2.82	0.42
1:A:143:ASN:HB2	9:I:48:PRO:HD2	2.01	0.42
1:N:351:GLU:O	1:N:355:LYS:HB2	2.20	0.42
3:P:129:PHE:CE1	13:P:3001:AZO:H223	2.55	0.42
4:Q:169:LEU:O	4:Q:169:LEU:HD23	2.20	0.42
5:R:74:ILE:HG22	5:R:91:TRP:CD1	2.54	0.42
1:A:140:GLU:OE2	9:I:50:LEU:N	2.39	0.42
4:D:186:VAL:O	4:D:190:LEU:HG	2.19	0.42
7:G:40:ARG:HD2	17:G:2004:CDL:OA4	2.19	0.42
8:H:50:THR:HG23	8:H:50:THR:O	2.19	0.42
1:N:170:THR:CG2	1:N:171:THR:N	2.82	0.42
2:O:96:LEU:HD13	2:O:109:VAL:HG12	2.01	0.42
2:O:222:GLN:O	2:O:223:PHE:CD2	2.72	0.42
12:P:502:HEM:HMC2	12:P:502:HEM:HBC2	2.01	0.42
2:B:47:ILE:HD11	2:B:116:VAL:CG1	2.50	0.42
4:D:211:ILE:HD13	4:D:211:ILE:HA	1.89	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:270:LEU:HA	1:N:270:LEU:HD23	1.88	0.42
1:A:206:LYS:HA	1:A:209:VAL:HG12	2.01	0.42
2:B:26:ILE:HG12	2:B:26:ILE:O	2.20	0.42
5:E:81:ILE:HG22	5:E:100:HIS:HB2	2.00	0.42
5:E:161:HIS:HB2	19:E:501:FES:S1	2.60	0.42
2:O:399:ALA:HA	2:O:402:ILE:HG22	2.01	0.42
3:P:70:THR:O	3:P:77:GLY:HA3	2.20	0.42
4:Q:240:PRO:O	4:Q:241:LYS:OXT	2.37	0.42
10:W:38:GLY:O	10:W:41:ALA:HB3	2.19	0.42
1:A:240:GLU:HA	1:A:422:LEU:O	2.20	0.42
2:B:162:ASN:O	2:B:244:ILE:HD12	2.20	0.42
3:C:9:HIS:CD2	3:C:11:LEU:HB2	2.55	0.42
1:N:41:ILE:HD13	1:N:190:PHE:CD2	2.55	0.42
2:O:341:MET:CE	2:O:417:PHE:HE2	2.23	0.42
2:O:54:GLY:O	2:O:56:ARG:N	2.53	0.42
3:P:288:LYS:O	3:P:292:VAL:HG23	2.19	0.42
4:Q:41:HIS:CE1	4:Q:110:PRO:HB2	2.54	0.42
1:A:19:LEU:HB2	1:A:21:ASN:OD1	2.20	0.42
2:B:166:ALA:HB2	2:B:244:ILE:HG13	2.02	0.42
2:B:345:LYS:HG2	2:B:418:VAL:HG13	2.02	0.42
2:B:50:PHE:CD1	2:B:50:PHE:N	2.88	0.42
1:N:111:GLU:HG3	1:N:215:HIS:NE2	2.35	0.42
1:N:51:LYS:HB2	1:N:51:LYS:HE3	1.91	0.42
2:O:54:GLY:C	2:O:56:ARG:N	2.73	0.42
3:P:342:GLN:NE2	3:P:342:GLN:HA	2.35	0.42
2:B:169:LYS:O	2:B:170:THR:HG23	2.19	0.41
2:B:246:GLU:HB3	2:B:427:SER:HB3	2.01	0.41
10:J:4:ALA:O	10:J:8:GLN:HG3	2.20	0.41
1:N:418:LYS:O	1:N:420:PRO:HD3	2.20	0.41
1:N:243:ALA:O	1:N:425:VAL:HA	2.20	0.41
2:O:67:HIS:O	2:O:70:ARG:HB3	2.19	0.41
9:V:52:ARG:HG3	9:V:52:ARG:HH11	1.85	0.41
1:A:271:HIS:CE1	1:A:311:ASN:HD22	2.38	0.41
1:A:281:ASP:O	1:A:283:THR:N	2.53	0.41
1:A:373:THR:HB	1:A:374:PRO:CD	2.50	0.41
2:B:54:GLY:C	2:B:56:ARG:N	2.73	0.41
3:C:130:VAL:HG23	3:C:183:HIS:HB2	2.01	0.41
3:C:31:TRP:NE1	11:C:2007:PEE:O4	2.53	0.41
3:C:28:ILE:CD1	14:C:2002:UQ:HM21	2.50	0.41
16:D:501:HEC:HAD1	16:D:501:HEC:HMD1	1.88	0.41
5:E:117:LEU:HD23	5:E:119:ASP:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:179:ASN:O	5:E:180:LEU:C	2.57	0.41
4:Q:223:LYS:C	4:Q:223:LYS:HD3	2.41	0.41
4:Q:68:VAL:HG11	4:Q:92:PRO:CG	2.50	0.41
1:A:206:LYS:HA	1:A:209:VAL:CG1	2.51	0.41
2:B:399:ALA:HA	2:B:402:ILE:HG22	2.02	0.41
2:B:59:THR:CG2	2:B:60:THR:N	2.83	0.41
3:C:233:LEU:O	3:C:237:LEU:HB2	2.20	0.41
10:J:7:ARG:NH1	10:J:7:ARG:CB	2.71	0.41
3:P:271:PRO:HB2	3:P:275:PHE:HB2	2.02	0.41
6:S:13:MET:HA	6:S:16:ILE:HD12	2.02	0.41
9:V:69:SER:HB2	9:V:72:ALA:H	1.84	0.41
2:B:361:LYS:HD3	2:B:403:ASP:HA	2.02	0.41
2:B:54:GLY:O	2:B:56:ARG:N	2.54	0.41
3:C:325:LEU:HD22	3:C:370:ILE:HG13	2.03	0.41
1:N:117:VAL:HG23	1:N:118:GLN:HG3	2.03	0.41
1:N:217:SER:O	1:N:218:GLY:C	2.59	0.41
1:N:3:THR:HG23	1:N:6:GLN:OE1	2.20	0.41
5:R:83:GLU:CD	5:R:102:THR:HA	2.40	0.41
9:V:35:UNK:CG	9:V:36:UNK:N	2.75	0.41
1:A:295:ALA:O	1:A:299:VAL:HG23	2.21	0.41
4:D:68:VAL:HG11	4:D:92:PRO:HG3	2.03	0.41
5:E:185:TYR:O	5:E:186:GLN:HB3	2.21	0.41
3:C:313:GLN:NE2	6:F:36:THR:OG1	2.48	0.41
1:N:106:MET:CE	1:N:110:VAL:HG21	2.50	0.41
1:N:163:LEU:HA	1:N:163:LEU:HD23	1.93	0.41
1:N:90:THR:O	1:N:167:VAL:HG11	2.21	0.41
2:O:37:SER:CB	2:O:213:HIS:ND1	2.68	0.41
5:R:185:TYR:CD2	5:R:185:TYR:N	2.88	0.41
2:B:29:LEU:HD12	2:B:33:LEU:HD23	2.02	0.41
2:B:385:GLU:C	2:B:387:LEU:H	2.24	0.41
3:C:242:THR:O	3:C:246:PHE:HB2	2.20	0.41
8:H:21:ARG:HD2	8:H:65:ARG:NH1	2.36	0.41
8:H:65:ARG:O	8:H:68:CYS:HB3	2.20	0.41
1:N:133:VAL:O	1:N:137:GLU:HG3	2.21	0.41
1:N:70:ARG:HA	1:N:71:PRO:HD2	1.80	0.41
3:P:271:PRO:HD2	3:P:279:TYR:CD2	2.55	0.41
3:P:49:GLY:O	12:P:501:HEM:HAC	2.20	0.41
5:R:161:HIS:HB2	19:R:501:FES:S1	2.61	0.41
9:V:32:UNK:N	9:V:73:PRO:HG2	2.36	0.41
1:A:106:MET:N	1:A:107:PRO:HD2	2.35	0.41
1:A:279:ARG:HH22	9:I:30:UNK:C	2.33	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:2:ILE:HG22	7:G:6:ASN:HD21	1.86	0.41
1:N:47:TYR:CZ	1:N:231:LEU:HD11	2.55	0.41
2:O:101:THR:OG1	2:O:104:LYS:HG3	2.20	0.41
2:O:227:ARG:O	2:O:228:SER:O	2.39	0.41
4:Q:74:PRO:HA	4:Q:79:GLU:O	2.21	0.41
5:R:75:GLU:HB3	5:R:194:VAL:HG22	2.01	0.41
5:R:76:ILE:CD1	5:R:98:VAL:HG21	2.51	0.41
4:D:220:TYR:O	4:D:224:ARG:HG2	2.20	0.41
5:E:102:THR:C	5:E:103:GLN:HG3	2.41	0.41
5:E:119:ASP:O	5:E:121:GLN:N	2.53	0.41
1:N:205:HIS:O	1:N:209:VAL:HG12	2.20	0.41
1:N:342:TRP:O	1:N:345:LEU:HB2	2.20	0.41
2:O:98:VAL:HA	2:O:106:THR:O	2.21	0.41
2:O:248:ASN:ND2	2:O:250:HIS:H	2.18	0.41
2:O:399:ALA:O	2:O:402:ILE:CG2	2.63	0.41
3:P:141:PHE:HE1	3:P:171:VAL:O	2.04	0.41
4:Q:165:TYR:CZ	4:Q:168:ILE:HG13	2.56	0.41
8:U:36:ARG:HB3	8:U:36:ARG:CZ	2.50	0.41
2:B:291:VAL:HA	2:B:297:GLN:NE2	2.36	0.41
2:B:355:GLU:CD	2:B:359:LYS:HE3	2.41	0.41
3:C:5:ILE:O	3:C:5:ILE:HG22	2.21	0.41
8:H:39:LEU:O	8:H:42:ALA:HB3	2.20	0.41
2:B:287:ARG:CB	9:I:53:GLU:HG3	2.51	0.41
2:O:306:PRO:HA	9:V:52:ARG:CG	2.50	0.41
1:A:106:MET:CE	1:A:110:VAL:HG21	2.50	0.41
1:A:189:HIS:ND1	1:A:194:ARG:NH2	2.65	0.41
1:A:351:GLU:O	1:A:355:LYS:HB2	2.20	0.41
2:B:22:GLU:O	2:B:23:ASP:CG	2.59	0.41
1:N:268:VAL:O	1:N:272:VAL:HG23	2.21	0.41
2:O:341:MET:HE2	2:O:341:MET:CA	2.45	0.41
4:Q:186:VAL:O	4:Q:190:LEU:HG	2.20	0.41
5:R:185:TYR:HD2	5:R:185:TYR:N	2.19	0.41
6:S:10:GLY:C	6:S:12:LEU:H	2.24	0.41
6:S:17:ARG:NH1	6:S:17:ARG:HG2	2.35	0.41
1:A:402:VAL:HG22	1:A:406:MET:HE1	2.01	0.41
1:A:422:LEU:HD22	1:A:437:ILE:HD13	2.03	0.41
2:B:257:VAL:HG22	2:B:424:MET:HG3	2.03	0.41
3:C:342:GLN:HA	3:C:342:GLN:NE2	2.35	0.41
5:E:75:GLU:HA	5:E:193:VAL:O	2.21	0.41
1:N:4:TYR:HE2	1:N:396:ASP:OD2	2.04	0.41
1:N:46:ARG:NH1	1:N:93:GLU:OE2	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:43:PRO:O	2:O:113:ARG:HG3	2.21	0.41
2:O:225:ASN:C	2:O:227:ARG:HG3	2.41	0.41
3:P:172:ASP:OD1	3:P:173:ASN:N	2.52	0.41
6:S:71:LYS:O	6:S:72:HIS:HB2	2.21	0.41
1:A:264:ASP:HA	1:A:265:PRO:HD3	1.82	0.40
3:C:272:GLU:O	3:C:273:TRP:C	2.59	0.40
4:D:116:ILE:HG12	16:D:501:HEC:HMA3	2.03	0.40
1:N:402:VAL:HA	1:N:406:MET:HE1	2.02	0.40
2:O:209:ILE:HG22	2:O:210:GLY:N	2.36	0.40
14:P:3002:UQ:HM51	14:P:3002:UQ:H8	2.02	0.40
1:A:37:VAL:HG22	1:A:109:VAL:HG11	2.03	0.40
1:A:422:LEU:HD22	1:A:437:ILE:CD1	2.51	0.40
2:B:141:GLN:N	2:B:142:PRO:HD2	2.35	0.40
4:D:158:ILE:HG12	4:D:160:MET:H	1.86	0.40
1:N:106:MET:HE2	1:N:110:VAL:HG23	2.02	0.40
1:N:264:ASP:HA	1:N:265:PRO:HD3	1.85	0.40
2:O:150:VAL:CG2	2:O:151:ALA:N	2.84	0.40
1:A:270:LEU:O	1:A:273:ALA:HB3	2.20	0.40
5:E:172:ARG:HB2	5:E:173:LYS:H	1.74	0.40
3:C:31:TRP:HE1	17:G:2004:CDL:H1	1.87	0.40
1:N:48:GLU:CD	1:N:54:GLY:H	2.24	0.40
2:O:297:GLN:O	2:O:301:LYS:HG3	2.21	0.40
2:O:403:ASP:C	2:O:405:VAL:H	2.24	0.40
4:Q:91:PHE:HA	4:Q:92:PRO:HD3	1.76	0.40
5:R:164:HIS:CD2	5:R:173:LYS:HB3	2.56	0.40
6:S:96:GLU:OE1	6:S:99:ARG:NH2	2.54	0.40
1:A:320:PHE:HE2	1:A:415:ILE:HD11	1.86	0.40
1:A:383:LEU:O	1:A:387:GLY:HA2	2.22	0.40
1:A:51:LYS:HB2	1:A:51:LYS:HE3	1.89	0.40
3:C:30:ALA:HB1	17:D:2003:CDL:H111	2.02	0.40
5:E:101:ARG:NH2	5:E:130:PRO:O	2.55	0.40
1:N:62:LEU:O	1:N:64:PHE:N	2.55	0.40
2:O:168:TYR:HB2	2:O:173:ALA:HB2	2.04	0.40
2:O:246:GLU:HB3	2:O:427:SER:HB3	2.02	0.40
2:O:172:LEU:HD13	2:O:316:TYR:CD1	2.56	0.40
5:R:141:HIS:HB3	19:R:501:FES:S2	2.62	0.40
2:O:307:PHE:HE2	9:V:52:ARG:HE	1.69	0.40
2:B:206:LEU:HG	2:B:206:LEU:O	2.22	0.40
7:G:29:ILE:HA	7:G:33:ALA:HB3	2.04	0.40
1:N:233:ARG:NH2	1:N:316:ASP:O	2.53	0.40
3:P:120:LEU:HA	3:P:120:LEU:HD23	1.88	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:501:HEC:CMB	16:Q:501:HEC:HBB3	2.51	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	442/446 (99%)	411 (93%)	25 (6%)	6 (1%)	13	37
1	N	440/446 (99%)	408 (93%)	25 (6%)	7 (2%)	11	33
2	B	418/441 (95%)	353 (84%)	50 (12%)	15 (4%)	4	12
2	O	420/441 (95%)	364 (87%)	42 (10%)	14 (3%)	4	14
3	C	378/380 (100%)	360 (95%)	14 (4%)	4 (1%)	17	44
3	P	377/380 (99%)	353 (94%)	19 (5%)	5 (1%)	14	39
4	D	239/241 (99%)	223 (93%)	16 (7%)	0	100	100
4	Q	239/241 (99%)	221 (92%)	16 (7%)	2 (1%)	22	53
5	E	194/196 (99%)	148 (76%)	34 (18%)	12 (6%)	2	4
5	R	194/196 (99%)	162 (84%)	23 (12%)	9 (5%)	3	8
6	F	99/110 (90%)	96 (97%)	2 (2%)	1 (1%)	18	47
6	S	99/110 (90%)	90 (91%)	8 (8%)	1 (1%)	18	47
7	G	78/81 (96%)	70 (90%)	7 (9%)	1 (1%)	14	39
7	T	77/81 (95%)	69 (90%)	6 (8%)	2 (3%)	6	19
8	H	68/77 (88%)	65 (96%)	3 (4%)	0	100	100
8	U	65/77 (84%)	61 (94%)	2 (3%)	2 (3%)	5	15
9	I	29/47 (62%)	27 (93%)	2 (7%)	0	100	100
9	V	29/47 (62%)	28 (97%)	1 (3%)	0	100	100
10	J	59/61 (97%)	56 (95%)	3 (5%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	W	58/61 (95%)	54 (93%)	3 (5%)	1 (2%)	11	31
All	All	4002/4160 (96%)	3619 (90%)	301 (8%)	82 (2%)	9	27

All (82) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	21	ALA
2	B	24	LEU
2	B	29	LEU
2	B	171	ALA
2	B	226	ILE
2	B	228	SER
3	C	287	ASN
5	E	102	THR
5	E	127	VAL
5	E	128	LYS
5	E	130	PRO
5	E	163	SER
1	N	282	ARG
2	O	171	ALA
2	O	222	GLN
2	O	228	SER
3	P	287	ASN
4	Q	3	LEU
5	R	163	SER
8	U	49	HIS
8	U	52	GLU
1	A	218	GLY
1	A	262	TRP
1	A	282	ARG
2	B	26	ILE
2	B	231	GLY
2	B	386	ALA
2	B	389	SER
5	E	80	ASP
5	E	177	PRO
5	E	191	ASP
1	N	218	GLY
1	N	262	TRP
2	O	26	ILE
2	O	231	GLY
2	O	372	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	O	389	SER
3	P	157	ILE
10	W	61	ALA
1	A	72	CYS
1	A	433	ASP
2	B	221	GLU
2	B	372	VAL
3	C	264	VAL
1	N	72	CYS
1	N	433	ASP
2	O	19	PRO
2	O	24	LEU
5	R	185	TYR
5	R	191	ASP
6	S	11	ARG
2	B	222	GLN
2	B	224	LEU
3	C	3	PRO
5	E	115	SER
1	N	63	ALA
2	O	319	SER
2	O	386	ALA
3	P	156	TYR
3	P	264	VAL
2	B	55	SER
1	N	443	TRP
2	O	55	SER
2	O	221	GLU
3	P	3	PRO
4	Q	177	ALA
5	R	127	VAL
7	T	33	ALA
5	E	137	GLY
6	F	77	LYS
5	R	113	ASP
5	R	120	PRO
5	R	177	PRO
7	T	50	PRO
3	C	158	GLY
5	E	120	PRO
5	R	137	GLY
7	G	50	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	O	208	GLY
1	A	71	PRO
5	E	154	GLY
5	R	154	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	365/368 (99%)	352 (96%)	13 (4%)	40	72
1	N	365/368 (99%)	352 (96%)	13 (4%)	40	72
2	B	331/347 (95%)	320 (97%)	11 (3%)	43	75
2	O	333/347 (96%)	323 (97%)	10 (3%)	46	78
3	C	328/329 (100%)	320 (98%)	8 (2%)	54	83
3	P	328/329 (100%)	322 (98%)	6 (2%)	64	88
4	D	200/200 (100%)	197 (98%)	3 (2%)	70	90
4	Q	200/200 (100%)	197 (98%)	3 (2%)	70	90
5	E	166/166 (100%)	162 (98%)	4 (2%)	54	83
5	R	165/166 (99%)	161 (98%)	4 (2%)	54	83
6	F	93/96 (97%)	90 (97%)	3 (3%)	44	76
6	S	93/96 (97%)	89 (96%)	4 (4%)	33	66
7	G	71/71 (100%)	70 (99%)	1 (1%)	71	91
7	T	70/71 (99%)	69 (99%)	1 (1%)	71	91
8	H	65/71 (92%)	65 (100%)	0	100	100
8	U	63/71 (89%)	62 (98%)	1 (2%)	68	90
9	I	23/26 (88%)	21 (91%)	2 (9%)	12	32
9	V	23/26 (88%)	20 (87%)	3 (13%)	5	13
10	J	49/49 (100%)	47 (96%)	2 (4%)	35	68
10	W	47/49 (96%)	47 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3378/3446 (98%)	3286 (97%)	92 (3%)	50 81

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	A	58	PHE
1	A	86	PHE
1	A	106	MET
1	A	179	ARG
1	A	181	ASP
1	A	281	ASP
1	A	307	PHE
1	A	352	SER
1	A	395	TRP
1	A	405	ARG
1	A	432	LEU
1	A	443	TRP
2	B	23	ASP
2	B	31	ASN
2	B	104	LYS
2	B	193	HIS
2	B	225	ASN
2	B	248	ASN
2	B	250	HIS
2	B	270	ASN
2	B	341	MET
2	B	402	ILE
2	B	437	ASP
3	C	22	LEU
3	C	41	CYS
3	C	81	ARG
3	C	91	PHE
3	C	184	PHE
3	C	223	PRO
3	C	240	PHE
3	C	367	PHE
4	D	70	VAL
4	D	169	LEU
4	D	203	ARG
5	E	52	LYS
5	E	131	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	E	178	TYR
5	E	185	TYR
6	F	52	GLU
6	F	64	ARG
6	F	70	LEU
7	G	28	ASN
9	I	68	ILE
9	I	71	ASN
10	J	59	TYR
10	J	60	GLU
1	N	18	THR
1	N	49	ASN
1	N	58	PHE
1	N	86	PHE
1	N	106	MET
1	N	181	ASP
1	N	281	ASP
1	N	307	PHE
1	N	352	SER
1	N	395	TRP
1	N	405	ARG
1	N	432	LEU
1	N	443	TRP
2	O	18	CYS
2	O	19	PRO
2	O	31	ASN
2	O	84	ARG
2	O	104	LYS
2	O	193	HIS
2	O	248	ASN
2	O	250	HIS
2	O	341	MET
2	O	402	ILE
3	P	81	ARG
3	P	91	PHE
3	P	184	PHE
3	P	240	PHE
3	P	256	ASN
3	P	367	PHE
4	Q	70	VAL
4	Q	169	LEU
4	Q	203	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	R	31	ASP
5	R	52	LYS
5	R	178	TYR
5	R	185	TYR
6	S	13	MET
6	S	52	GLU
6	S	64	ARG
6	S	70	LEU
7	T	28	ASN
8	U	49	HIS
9	V	58	ARG
9	V	68	ILE
9	V	75	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (86) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	49	ASN
1	A	85	HIS
1	A	118	GLN
1	A	173	ASN
1	A	267	ASN
1	A	274	ASN
1	A	289	HIS
1	A	308	GLN
1	A	311	ASN
1	A	339	GLN
2	B	31	ASN
2	B	153	GLN
2	B	156	GLN
2	B	247	GLN
2	B	248	ASN
2	B	270	ASN
2	B	276	GLN
2	B	297	GLN
2	B	329	GLN
2	B	343	GLN
2	B	362	ASN
2	B	363	GLN
3	C	9	HIS
3	C	17	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	69	HIS
3	C	82	ASN
3	C	207	ASN
3	C	313	GLN
3	C	332	ASN
3	C	342	GLN
4	D	35	GLN
4	D	50	ASN
4	D	148	HIS
5	E	3	ASN
5	E	122	HIS
5	E	149	ASN
5	E	164	HIS
7	G	6	ASN
7	G	23	GLN
7	G	44	GLN
7	G	73	ASN
9	I	71	ASN
1	N	32	GLN
1	N	49	ASN
1	N	85	HIS
1	N	118	GLN
1	N	143	ASN
1	N	173	ASN
1	N	267	ASN
1	N	274	ASN
1	N	289	HIS
1	N	308	GLN
1	N	311	ASN
1	N	339	GLN
2	O	31	ASN
2	O	153	GLN
2	O	156	GLN
2	O	247	GLN
2	O	248	ASN
2	O	276	GLN
2	O	297	GLN
2	O	329	GLN
2	O	343	GLN
2	O	362	ASN
2	O	363	GLN
3	P	9	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	P	17	ASN
3	P	69	HIS
3	P	82	ASN
3	P	207	ASN
3	P	313	GLN
3	P	332	ASN
3	P	342	GLN
4	Q	35	GLN
4	Q	50	ASN
4	Q	148	HIS
4	Q	200	GLN
5	R	57	GLN
5	R	107	ASN
5	R	164	HIS
5	R	186	GLN
7	T	23	GLN
7	T	44	GLN
7	T	73	ASN
7	T	79	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

29 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
11	PEE	A	2005	-	49,49,50	1.44	9 (18%)	51,54,55	0.96	5 (9%)
11	PEE	A	2008	-	20,20,50	1.81	6 (30%)	22,25,55	0.70	0
13	AZO	C	2001	-	32,32,32	2.99	16 (50%)	40,42,42	3.27	11 (27%)
14	UQ	C	2002	-	19,19,63	2.57	10 (52%)	23,26,79	1.31	3 (13%)
11	PEE	C	2007	-	48,48,50	1.29	6 (12%)	50,53,55	0.93	5 (10%)
15	GOL	C	2011	-	5,5,5	1.37	0	5,5,5	0.63	0
12	HEM	C	501	3	28,50,50	2.00	8 (28%)	17,82,82	1.62	6 (35%)
12	HEM	C	502	3	28,50,50	2.07	8 (28%)	17,82,82	1.64	4 (23%)
17	CDL	D	2003	-	41,41,99	1.17	2 (4%)	43,53,111	1.08	2 (4%)
18	BOG	D	2009	-	20,20,20	1.04	2 (10%)	25,25,25	0.84	2 (8%)
18	BOG	D	2091	-	13,13,20	1.31	2 (15%)	18,18,25	1.11	2 (11%)
16	HEC	D	501	4	28,50,50	2.26	5 (17%)	16,82,82	1.11	1 (6%)
19	FES	E	501	5	0,4,4	0.00	-	0,4,4	0.00	-
17	CDL	G	2004	-	39,39,99	1.20	2 (5%)	41,51,111	1.15	3 (7%)
11	PEE	N	3008	-	4,4,50	3.58	4 (100%)	6,6,55	0.55	0
18	BOG	P	2010	-	12,12,20	1.39	3 (25%)	17,17,25	0.62	0
13	AZO	P	3001	-	32,32,32	3.19	17 (53%)	40,42,42	3.30	13 (32%)
14	UQ	P	3002	-	19,19,63	2.55	10 (52%)	23,26,79	1.27	3 (13%)
11	PEE	P	3005	-	49,49,50	1.42	9 (18%)	51,54,55	0.96	5 (9%)
11	PEE	P	3007	-	48,48,50	1.23	7 (14%)	50,53,55	0.90	4 (8%)
15	GOL	P	3011	-	5,5,5	1.38	0	5,5,5	0.65	0
12	HEM	P	501	3	28,50,50	1.99	9 (32%)	17,82,82	1.55	3 (17%)
12	HEM	P	502	3	28,50,50	2.02	7 (25%)	17,82,82	1.57	2 (11%)
17	CDL	Q	3003	-	41,41,99	1.18	2 (4%)	43,53,111	1.10	4 (9%)
18	BOG	Q	3009	-	20,20,20	1.00	1 (5%)	25,25,25	0.81	1 (4%)
18	BOG	Q	3091	-	13,13,20	1.37	2 (15%)	18,18,25	1.13	2 (11%)
16	HEC	Q	501	4	28,50,50	2.26	3 (10%)	16,82,82	1.21	2 (12%)
19	FES	R	501	5	0,4,4	0.00	-	0,4,4	0.00	-
17	CDL	T	3004	-	39,39,99	1.20	2 (5%)	41,51,111	1.16	4 (9%)

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
11	PEE	A	2005	-	-	0/53/53/54	0/0/0/0
11	PEE	A	2008	-	-	0/24/24/54	0/0/0/0
13	AZO	C	2001	-	-	0/23/23/23	0/3/3/3
14	UQ	C	2002	-	-	0/11/35/87	0/1/1/1
11	PEE	C	2007	-	-	0/52/52/54	0/0/0/0
15	GOL	C	2011	-	-	0/4/4/4	0/0/0/0
12	HEM	C	501	3	-	0/6/54/54	0/0/8/8
12	HEM	C	502	3	-	0/6/54/54	0/0/8/8
17	CDL	D	2003	-	-	0/51/51/110	0/0/0/0
18	BOG	D	2009	-	-	0/11/31/31	0/1/1/1
18	BOG	D	2091	-	-	0/4/24/31	0/1/1/1
16	HEC	D	501	4	-	0/6/54/54	0/0/8/8
19	FES	E	501	5	-	0/0/4/4	0/1/1/1
17	CDL	G	2004	-	-	0/49/49/110	0/0/0/0
11	PEE	N	3008	-	-	0/0/0/54	0/0/0/0
18	BOG	P	2010	-	-	0/2/22/31	0/1/1/1
13	AZO	P	3001	-	-	0/23/23/23	0/3/3/3
14	UQ	P	3002	-	-	0/11/35/87	0/1/1/1
11	PEE	P	3005	-	-	0/53/53/54	0/0/0/0
11	PEE	P	3007	-	-	0/52/52/54	0/0/0/0
15	GOL	P	3011	-	-	0/4/4/4	0/0/0/0
12	HEM	P	501	3	-	0/6/54/54	0/0/8/8
12	HEM	P	502	3	-	0/6/54/54	0/0/8/8
17	CDL	Q	3003	-	-	0/51/51/110	0/0/0/0
18	BOG	Q	3009	-	-	0/11/31/31	0/1/1/1
18	BOG	Q	3091	-	-	0/4/24/31	0/1/1/1
16	HEC	Q	501	4	-	0/6/54/54	0/0/8/8
19	FES	R	501	5	-	0/0/4/4	0/1/1/1
17	CDL	T	3004	-	-	0/49/49/110	0/0/0/0

All (152) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	D	501	HEC	C3B-C2B	-8.67	1.31	1.40
16	Q	501	HEC	C3B-C2B	-8.64	1.31	1.40
16	Q	501	HEC	C3C-C2C	-6.77	1.33	1.40
13	P	3001	AZO	C18-C19	-6.47	1.32	1.48
13	C	2001	AZO	C18-C19	-6.18	1.33	1.48
16	D	501	HEC	C3C-C2C	-6.02	1.34	1.40
12	C	501	HEM	C3B-CAB	-4.48	1.39	1.47
12	P	502	HEM	C3B-CAB	-4.43	1.39	1.47
12	P	502	HEM	C3B-C2B	-4.29	1.34	1.40
12	C	502	HEM	C3B-CAB	-4.15	1.39	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	502	HEM	C3C-C2C	-4.02	1.35	1.40
12	C	502	HEM	C3C-CAC	-4.02	1.39	1.47
12	C	501	HEM	C3C-CAC	-3.92	1.39	1.47
12	P	502	HEM	C3C-CAC	-3.87	1.40	1.47
12	P	501	HEM	C3B-CAB	-3.71	1.40	1.47
12	P	501	HEM	C3C-CAC	-3.39	1.41	1.47
11	P	3005	PEE	C19-C18	-3.00	1.34	1.51
12	P	501	HEM	C3B-C2B	-2.99	1.36	1.40
11	A	2005	PEE	C19-C18	-2.95	1.34	1.51
12	P	501	HEM	C3C-C2C	-2.95	1.36	1.40
11	P	3007	PEE	C22-C21	-2.89	1.35	1.51
11	P	3007	PEE	C19-C18	-2.82	1.35	1.51
11	P	3005	PEE	C22-C21	-2.82	1.35	1.51
11	C	2007	PEE	C19-C18	-2.81	1.35	1.51
11	A	2005	PEE	C22-C21	-2.77	1.35	1.51
16	D	501	HEC	C1D-CHD	-2.69	1.33	1.40
11	C	2007	PEE	C22-C21	-2.67	1.36	1.51
16	D	501	HEC	C4C-NC	-2.52	1.33	1.36
16	Q	501	HEC	C1D-CHD	-2.52	1.33	1.40
17	T	3004	CDL	OB2-CB2	-2.12	1.36	1.44
16	D	501	HEC	C4B-NB	-2.02	1.34	1.36
18	D	2009	BOG	C1-C2	2.02	1.58	1.52
13	C	2001	AZO	C15-C14	2.04	1.43	1.38
11	P	3007	PEE	C3-C2	2.05	1.56	1.50
13	C	2001	AZO	C17-C18	2.06	1.51	1.49
11	P	3007	PEE	C31-C30	2.06	1.56	1.50
17	D	2003	CDL	CA3-CA4	2.06	1.56	1.50
13	P	3001	AZO	C17-C18	2.07	1.51	1.49
13	C	2001	AZO	C5-C6	2.07	1.42	1.38
17	D	2003	CDL	O1-C1	2.07	1.49	1.43
13	P	3001	AZO	C9-C10	2.07	1.42	1.38
13	P	3001	AZO	C15-C14	2.07	1.43	1.38
17	Q	3003	CDL	CA3-CA4	2.09	1.56	1.50
17	G	2004	CDL	O1-C1	2.13	1.49	1.43
18	P	2010	BOG	C1-C2	2.13	1.57	1.52
11	N	3008	PEE	P-O2P	2.13	1.61	1.54
12	C	502	HEM	CMD-C2D	2.13	1.56	1.51
13	C	2001	AZO	O5-C21	2.14	1.38	1.34
17	G	2004	CDL	CB3-CB4	2.17	1.56	1.50
13	P	3001	AZO	C13-C12	2.18	1.44	1.39
11	A	2008	PEE	C11-C10	2.19	1.57	1.50
17	T	3004	CDL	O1-C1	2.20	1.50	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	D	2091	BOG	C4-C5	2.23	1.57	1.53
17	Q	3003	CDL	O1-C1	2.25	1.50	1.43
13	P	3001	AZO	O2-C10	2.26	1.39	1.36
18	Q	3091	BOG	C4-C5	2.27	1.57	1.53
18	P	2010	BOG	C4-C5	2.27	1.57	1.53
11	P	3005	PEE	C11-C10	2.28	1.57	1.50
11	C	2007	PEE	C3-C2	2.30	1.57	1.50
11	A	2005	PEE	C11-C10	2.32	1.57	1.50
11	P	3005	PEE	C31-C30	2.33	1.57	1.50
12	C	501	HEM	C4D-ND	2.35	1.39	1.36
11	P	3005	PEE	C1-C2	2.39	1.57	1.50
12	P	501	HEM	C1D-ND	2.40	1.41	1.36
12	C	501	HEM	C1D-ND	2.41	1.41	1.36
18	D	2091	BOG	O5-C1	2.42	1.47	1.41
13	P	3001	AZO	C15-C16	2.42	1.43	1.38
18	Q	3009	BOG	O5-C1	2.43	1.47	1.41
12	C	502	HEM	C4C-NC	2.43	1.39	1.36
18	D	2009	BOG	O5-C1	2.47	1.48	1.41
14	P	3002	UQ	CM5-C5	2.47	1.56	1.50
18	P	2010	BOG	O5-C1	2.48	1.47	1.43
13	P	3001	AZO	C4-C3	2.49	1.43	1.38
14	P	3002	UQ	C5-C4	2.49	1.56	1.47
14	C	2002	UQ	C5-C4	2.50	1.56	1.47
13	P	3001	AZO	C6-C7	2.51	1.44	1.39
12	C	502	HEM	CBC-CAC	2.51	1.46	1.28
14	C	2002	UQ	C7-C8	2.51	1.54	1.50
11	A	2005	PEE	C1-C2	2.52	1.57	1.50
13	C	2001	AZO	C15-C16	2.53	1.43	1.38
18	Q	3091	BOG	O5-C1	2.56	1.48	1.41
14	C	2002	UQ	C3-C4	2.56	1.56	1.48
11	A	2008	PEE	C1-C2	2.56	1.58	1.50
14	C	2002	UQ	CM5-C5	2.57	1.56	1.50
14	P	3002	UQ	C7-C8	2.58	1.54	1.50
14	P	3002	UQ	O2-C2	2.59	1.43	1.36
12	P	501	HEM	C4C-NC	2.59	1.39	1.36
11	P	3007	PEE	O2-C10	2.59	1.41	1.34
11	A	2005	PEE	C3-C2	2.60	1.58	1.50
11	A	2005	PEE	C31-C30	2.60	1.58	1.50
11	A	2008	PEE	C3-C2	2.60	1.58	1.50
13	C	2001	AZO	C5-C4	2.61	1.44	1.38
14	P	3002	UQ	C3-C4	2.62	1.56	1.48
14	C	2002	UQ	O2-C2	2.63	1.43	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	P	3005	PEE	C3-C2	2.64	1.58	1.50
13	P	3001	AZO	C5-C4	2.65	1.44	1.38
11	P	3007	PEE	P-O1P	2.67	1.60	1.50
13	C	2001	AZO	C6-C7	2.68	1.45	1.39
12	C	501	HEM	C4C-NC	2.71	1.40	1.36
14	P	3002	UQ	C2-C1	2.73	1.56	1.48
13	C	2001	AZO	C13-C12	2.76	1.45	1.39
11	C	2007	PEE	O2-C10	2.80	1.42	1.34
11	C	2007	PEE	P-O1P	2.84	1.61	1.50
11	N	3008	PEE	P-O3P	2.86	1.64	1.54
12	P	502	HEM	CBC-CAC	2.88	1.49	1.28
11	A	2008	PEE	P-O1P	2.94	1.61	1.50
11	A	2005	PEE	P-O1P	3.00	1.62	1.50
11	P	3005	PEE	P-O1P	3.01	1.62	1.50
13	C	2001	AZO	C4-C3	3.04	1.44	1.38
14	C	2002	UQ	C2-C1	3.04	1.57	1.48
14	C	2002	UQ	O3-C3	3.05	1.44	1.36
11	N	3008	PEE	P-O4P	3.05	1.65	1.54
11	P	3007	PEE	O3-C30	3.06	1.42	1.33
12	C	501	HEM	CBB-CAB	3.08	1.50	1.28
11	A	2008	PEE	O2-C10	3.09	1.43	1.34
13	P	3001	AZO	O5-C21	3.12	1.40	1.34
12	C	501	HEM	CBC-CAC	3.13	1.50	1.28
11	C	2007	PEE	O3-C30	3.14	1.42	1.33
11	A	2005	PEE	O2-C10	3.19	1.43	1.34
11	A	2008	PEE	O3-C30	3.24	1.42	1.33
12	P	501	HEM	CBC-CAC	3.25	1.51	1.28
12	P	502	HEM	C4C-NC	3.26	1.40	1.36
12	P	502	HEM	CBB-CAB	3.27	1.51	1.28
14	P	3002	UQ	O3-C3	3.27	1.45	1.36
12	P	501	HEM	CBB-CAB	3.29	1.52	1.28
11	P	3005	PEE	O3-C30	3.32	1.43	1.33
11	P	3005	PEE	O2-C10	3.43	1.44	1.34
12	P	502	HEM	C1B-NB	3.46	1.40	1.36
11	A	2005	PEE	O3-C30	3.50	1.43	1.33
13	C	2001	AZO	C8-N2	3.73	1.37	1.32
12	C	502	HEM	CBB-CAB	3.77	1.55	1.28
14	C	2002	UQ	C6-C1	3.78	1.57	1.46
14	P	3002	UQ	C6-C1	3.87	1.57	1.46
14	P	3002	UQ	C6-C5	3.91	1.43	1.35
13	C	2001	AZO	C10-N3	3.96	1.38	1.32
14	C	2002	UQ	C6-C5	4.08	1.44	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	P	501	HEM	C1B-NB	4.13	1.41	1.36
13	P	3001	AZO	C8-N2	4.36	1.38	1.32
12	C	502	HEM	C1B-NB	4.38	1.41	1.36
12	C	501	HEM	C1B-NB	4.44	1.42	1.36
13	P	3001	AZO	C10-N3	5.20	1.39	1.32
13	C	2001	AZO	C17-C12	5.23	1.50	1.40
14	C	2002	UQ	C7-C6	5.31	1.60	1.51
14	P	3002	UQ	C7-C6	5.41	1.60	1.51
11	N	3008	PEE	P-O1P	5.42	1.62	1.50
13	C	2001	AZO	C2-C7	5.43	1.52	1.40
13	P	3001	AZO	O4-C19	5.45	1.45	1.33
13	P	3001	AZO	C2-C7	5.79	1.53	1.40
13	C	2001	AZO	O4-C19	5.83	1.46	1.33
13	P	3001	AZO	C17-C12	5.92	1.51	1.40
13	C	2001	AZO	C21-C18	7.29	1.50	1.35
13	P	3001	AZO	C21-C18	7.65	1.51	1.35

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	C	2001	AZO	N2-C11-N3	-6.25	118.50	128.65
13	P	3001	AZO	N2-C11-N3	-5.98	118.93	128.65
13	C	2001	AZO	C22-O5-C21	-5.96	108.29	115.71
13	P	3001	AZO	C22-O5-C21	-5.95	108.29	115.71
12	P	502	HEM	C4C-C3C-C2C	-3.92	104.16	106.90
12	C	502	HEM	C4C-C3C-C2C	-3.81	104.23	106.90
13	P	3001	AZO	C9-C10-N3	-3.78	119.36	124.79
13	C	2001	AZO	C9-C10-N3	-3.48	119.79	124.79
17	T	3004	CDL	CB4-OB6-CB5	-3.37	109.91	117.88
12	P	501	HEM	C1D-C2D-C3D	-3.24	104.74	107.00
13	P	3001	AZO	C9-C8-N2	-3.23	120.15	124.79
17	G	2004	CDL	CA4-OA6-CA5	-3.17	110.39	117.88
16	D	501	HEC	CAA-C2A-C3A	-3.16	119.98	129.00
17	G	2004	CDL	CB4-OB6-CB5	-3.12	110.50	117.88
14	C	2002	UQ	C7-C6-C1	-3.08	114.54	118.47
16	Q	501	HEC	CAA-C2A-C3A	-3.07	120.23	129.00
13	C	2001	AZO	C9-C8-N2	-2.87	120.67	124.79
14	P	3002	UQ	C7-C6-C1	-2.75	114.95	118.47
17	T	3004	CDL	CA4-OA6-CA5	-2.74	111.41	117.88
12	P	502	HEM	CMD-C2D-C1D	-2.68	124.34	128.46
12	C	502	HEM	C1D-C2D-C3D	-2.60	105.19	107.00
17	D	2003	CDL	CB4-OB6-CB5	-2.60	111.74	117.88

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	C	501	HEM	CMA-C3A-C4A	-2.54	124.57	128.46
12	P	501	HEM	CAD-C3D-C2D	-2.46	121.97	129.00
17	Q	3003	CDL	CB4-OB6-CB5	-2.46	112.05	117.88
17	T	3004	CDL	CA6-CA4-CA3	-2.39	106.47	111.86
17	D	2003	CDL	CA6-CA4-CA3	-2.38	106.48	111.86
17	Q	3003	CDL	CA6-CA4-CA3	-2.34	106.58	111.86
12	C	501	HEM	C1D-C2D-C3D	-2.32	105.38	107.00
17	G	2004	CDL	CA6-CA4-CA3	-2.25	106.78	111.86
17	Q	3003	CDL	CA4-OA6-CA5	-2.18	112.73	117.88
14	P	3002	UQ	C10-C9-C8	-2.17	117.89	123.69
13	P	3001	AZO	O4-C19-O3	-2.12	119.41	123.54
17	T	3004	CDL	CB6-CB4-CB3	-2.10	107.11	111.86
14	C	2002	UQ	C10-C9-C8	-2.10	118.09	123.69
12	C	501	HEM	CAD-C3D-C2D	-2.07	123.09	129.00
17	Q	3003	CDL	CB6-CB4-CB3	-2.05	107.24	111.86
13	C	2001	AZO	O4-C19-O3	-2.00	119.63	123.54
12	C	502	HEM	CAD-C3D-C2D	-2.00	123.28	129.00
18	D	2009	BOG	O1-C1-C2	2.08	111.63	108.23
16	Q	501	HEC	CBA-CAA-C2A	2.09	116.45	112.47
11	C	2007	PEE	O3-C3-C2	2.15	114.06	108.66
13	P	3001	AZO	O2-C10-N3	2.15	123.04	119.05
12	C	502	HEM	CMB-C2B-C3B	2.16	128.91	124.89
12	C	501	HEM	C3B-C4B-NB	2.19	112.04	109.21
13	C	2001	AZO	C20-O4-C19	2.30	120.23	115.87
12	C	501	HEM	CMA-C3A-C2A	2.32	129.32	124.94
11	P	3005	PEE	C23-C22-C21	2.34	126.51	114.45
12	P	501	HEM	CMB-C2B-C3B	2.36	129.27	124.89
11	P	3007	PEE	C22-C21-C20	2.37	126.66	114.45
11	P	3007	PEE	C23-C22-C21	2.37	126.68	114.45
11	A	2005	PEE	C23-C22-C21	2.40	126.80	114.45
11	C	2007	PEE	C22-C21-C20	2.44	127.05	114.45
18	Q	3091	BOG	O1-C1-C2	2.47	111.08	108.14
11	A	2005	PEE	O3-C3-C2	2.49	114.91	108.66
11	C	2007	PEE	C23-C22-C21	2.51	127.39	114.45
11	C	2007	PEE	C19-C18-C17	2.52	127.44	114.45
11	P	3005	PEE	C22-C21-C20	2.53	127.47	114.45
13	P	3001	AZO	C10-C9-C8	2.54	117.67	115.20
18	D	2091	BOG	O1-C1-C2	2.54	111.16	108.14
11	A	2005	PEE	C22-C21-C20	2.54	127.56	114.45
11	P	3007	PEE	C19-C18-C17	2.55	127.57	114.45
11	P	3005	PEE	C19-C18-C17	2.55	127.61	114.45
11	P	3005	PEE	O3-C3-C2	2.58	115.14	108.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	2005	PEE	C19-C18-C17	2.60	127.83	114.45
11	A	2005	PEE	C20-C19-C18	2.64	128.03	114.45
11	P	3005	PEE	C20-C19-C18	2.66	128.19	114.45
13	P	3001	AZO	C12-O2-C10	2.67	124.74	118.48
18	D	2009	BOG	C1'-O1-C1	2.70	118.50	113.87
13	P	3001	AZO	C20-O4-C19	2.71	121.01	115.87
18	Q	3009	BOG	C1'-O1-C1	2.74	118.56	113.87
11	P	3007	PEE	C20-C19-C18	2.76	128.68	114.45
13	P	3001	AZO	C7-O1-C8	2.77	124.99	118.48
11	C	2007	PEE	C20-C19-C18	2.80	128.87	114.45
13	C	2001	AZO	C7-O1-C8	2.80	125.06	118.48
12	C	501	HEM	CMB-C2B-C3B	2.84	130.16	124.89
13	C	2001	AZO	C12-O2-C10	2.85	125.16	118.48
18	D	2091	BOG	C1'-O1-C1	3.34	118.50	113.29
18	Q	3091	BOG	C1'-O1-C1	3.53	118.80	113.29
14	P	3002	UQ	C8-C7-C6	3.88	122.76	111.85
14	C	2002	UQ	C8-C7-C6	3.95	122.94	111.85
13	P	3001	AZO	O4-C19-C18	4.80	119.53	111.91
13	C	2001	AZO	O4-C19-C18	4.86	119.61	111.91
13	C	2001	AZO	C11-N2-C8	11.23	121.79	114.32
13	P	3001	AZO	C11-N2-C8	11.36	121.88	114.32
13	P	3001	AZO	C11-N3-C10	11.55	122.00	114.32
13	C	2001	AZO	C11-N3-C10	11.79	122.16	114.32

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

21 monomers are involved in 54 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	C	2002	UQ	4	0
11	C	2007	PEE	5	0
15	C	2011	GOL	1	0
12	C	501	HEM	3	0
12	C	502	HEM	2	0
17	D	2003	CDL	4	0
18	D	2091	BOG	1	0
16	D	501	HEC	3	0
19	E	501	FES	2	0
17	G	2004	CDL	4	0
18	P	2010	BOG	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	P	3001	AZO	2	0
14	P	3002	UQ	6	0
11	P	3007	PEE	3	0
12	P	501	HEM	2	0
12	P	502	HEM	2	0
17	Q	3003	CDL	3	0
18	Q	3091	BOG	1	0
16	Q	501	HEC	2	0
19	R	501	FES	2	0
17	T	3004	CDL	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	444/446 (99%)	0.35	14 (3%)	48	38	41, 68, 96, 110	0
1	N	442/446 (99%)	0.34	14 (3%)	48	38	48, 80, 103, 110	0
2	B	420/441 (95%)	0.38	21 (5%)	30	21	57, 87, 120, 142	0
2	O	422/441 (95%)	0.37	16 (3%)	41	31	49, 85, 113, 129	0
3	C	380/380 (100%)	0.35	9 (2%)	59	50	30, 48, 88, 132	0
3	P	379/380 (99%)	0.36	14 (3%)	42	32	33, 63, 94, 132	0
4	D	241/241 (100%)	0.27	4 (1%)	70	64	36, 51, 88, 109	0
4	Q	241/241 (100%)	0.26	5 (2%)	64	56	56, 76, 106, 127	0
5	E	196/196 (100%)	1.68	69 (35%)	0	0	41, 144, 176, 184	0
5	R	196/196 (100%)	0.28	8 (4%)	38	28	51, 97, 144, 156	0
6	F	101/110 (91%)	0.21	0	100	100	38, 52, 70, 104	0
6	S	101/110 (91%)	0.07	0	100	100	60, 74, 107, 131	0
7	G	80/81 (98%)	0.45	2 (2%)	58	49	42, 61, 106, 117	0
7	T	79/81 (97%)	0.57	6 (7%)	15	8	56, 85, 150, 159	0
8	H	70/77 (90%)	0.39	1 (1%)	75	70	45, 68, 91, 128	0
8	U	67/77 (87%)	0.28	5 (7%)	15	9	90, 117, 137, 141	0
9	I	31/47 (65%)	1.83	13 (41%)	0	0	80, 115, 142, 143	0
9	V	31/47 (65%)	1.74	15 (48%)	0	0	78, 115, 140, 145	0
10	J	61/61 (100%)	0.19	2 (3%)	47	37	52, 65, 103, 147	0
10	W	60/61 (98%)	0.35	2 (3%)	47	37	63, 79, 109, 119	0
All	All	4042/4160 (97%)	0.42	220 (5%)	26	18	30, 73, 131, 184	0

All (220) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	E	157	TYR	7.7
5	E	109	GLU	7.3
5	E	188	VAL	7.0
5	E	116	LYS	6.6
5	E	98	VAL	6.4
9	I	63	ASP	6.3
5	E	117	LEU	6.0
9	V	63	ASP	5.8
2	B	220	ALA	5.7
5	E	84	GLY	5.6
9	I	48	PRO	5.6
5	R	196	GLY	5.5
4	D	241	LYS	5.5
5	E	159	PRO	5.5
2	B	33	LEU	5.4
7	T	78	GLU	5.3
9	I	50	LEU	5.2
5	E	171	ILE	5.1
5	E	163	SER	5.1
5	E	114	VAL	5.1
5	E	183	PRO	5.0
5	R	81	ILE	4.9
5	E	138	VAL	4.9
5	E	120	PRO	4.9
7	T	2	ILE	4.8
5	E	115	SER	4.7
5	E	102	THR	4.7
2	B	224	LEU	4.7
5	E	107	ASN	4.7
5	E	149	ASN	4.6
5	E	103	GLN	4.6
5	E	112	VAL	4.6
5	E	148	ALA	4.5
9	V	68	ILE	4.4
2	B	226	ILE	4.4
5	E	174	GLY	4.3
5	E	156	TYR	4.3
5	E	158	CYS	4.2
5	E	124	LEU	4.2
5	E	167	ALA	4.2
1	N	379	ILE	4.1
5	E	113	ASP	4.1
5	E	173	LYS	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	E	86	ASN	4.0
5	E	152	ASP	4.0
5	E	180	LEU	4.0
5	E	150	SER	3.9
5	E	165	TYR	3.9
1	N	127	ILE	3.9
5	E	108	GLN	3.9
7	T	77	TYR	3.7
5	E	178	TYR	3.7
10	J	63	GLU	3.7
9	I	76	VAL	3.7
4	Q	206	LEU	3.6
5	E	104	ALA	3.6
9	I	55	MET	3.6
9	I	51	CYS	3.5
8	U	13	LEU	3.5
5	E	145	VAL	3.5
4	Q	210	LEU	3.5
2	B	29	LEU	3.4
4	D	240	PRO	3.4
2	O	410	VAL	3.4
2	B	225	ASN	3.4
5	E	169	GLY	3.4
5	E	146	PRO	3.3
9	V	53	GLU	3.3
2	O	402	ILE	3.3
5	E	111	GLU	3.2
5	E	172	ARG	3.2
3	C	380	TYR	3.2
5	E	177	PRO	3.2
9	I	54	SER	3.2
1	N	122	LEU	3.2
9	V	54	SER	3.2
5	E	134	ILE	3.2
5	R	86	ASN	3.2
5	E	97	PHE	3.2
1	A	392	LEU	3.1
2	B	439	LEU	3.1
3	P	237	LEU	3.1
9	V	56	SER	3.1
5	E	168	SER	3.1
2	O	144	LEU	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	E	187	PHE	3.0
5	E	83	GLU	3.0
5	E	105	GLU	3.0
9	V	48	PRO	3.0
2	B	35	ILE	3.0
1	A	365	MET	3.0
4	Q	209	LEU	3.0
1	A	197	LEU	2.9
2	O	132	PHE	2.9
5	E	125	ASP	2.9
2	O	191	LEU	2.9
5	E	118	ARG	2.9
1	N	138	LEU	2.9
7	T	53	LEU	2.9
3	P	233	LEU	2.9
5	E	87	VAL	2.9
3	P	363	LEU	2.9
7	G	14	ILE	2.8
1	A	379	ILE	2.8
2	B	201	SER	2.8
2	O	352	VAL	2.8
7	T	6	ASN	2.8
1	A	216	PHE	2.8
1	N	386	TYR	2.8
3	C	345	GLU	2.8
9	I	64	LEU	2.8
9	I	77	ARG	2.7
1	N	376	CYS	2.7
3	C	236	MET	2.7
5	E	181	GLU	2.7
2	B	216	LEU	2.7
2	O	344	LEU	2.7
4	D	3	LEU	2.7
5	E	90	LYS	2.6
5	E	119	ASP	2.6
5	E	143	GLY	2.6
3	P	34	PHE	2.6
2	B	402	ILE	2.6
2	O	296	TYR	2.6
4	D	1	GLY	2.6
3	P	277	PHE	2.6
5	R	171	ILE	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	N	174	ILE	2.6
9	V	58	ARG	2.6
5	E	106	ILE	2.5
5	E	144	CYS	2.5
5	E	136	VAL	2.5
9	V	74	ALA	2.5
5	E	147	ILE	2.5
1	N	302	LYS	2.5
2	O	68	LEU	2.5
3	C	4	ASN	2.5
1	N	392	LEU	2.5
2	B	369	LEU	2.5
9	I	59	SER	2.4
1	N	182	LEU	2.4
2	O	355	GLU	2.4
2	B	386	ALA	2.4
9	V	55	MET	2.4
9	V	60	ALA	2.4
1	A	28	GLU	2.4
8	U	37	LEU	2.4
10	W	39	ALA	2.4
2	B	368	TYR	2.4
1	A	86	PHE	2.4
3	C	155	PRO	2.4
5	R	1	VAL	2.4
1	A	208	LEU	2.4
2	O	405	VAL	2.4
3	C	90	PHE	2.4
1	A	203	ILE	2.4
2	B	223	PHE	2.4
9	V	72	ALA	2.4
2	B	144	LEU	2.4
1	A	177	LEU	2.4
3	P	334	LEU	2.4
5	E	135	LEU	2.4
5	E	176	ALA	2.3
1	A	122	LEU	2.3
9	I	53	GLU	2.3
5	R	49	TYR	2.3
3	C	233	LEU	2.3
5	E	140	THR	2.3
2	B	157	VAL	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	N	349	THR	2.3
3	P	91	PHE	2.3
5	E	99	ARG	2.3
5	E	89	PHE	2.3
9	V	47	ARG	2.3
5	E	88	ALA	2.2
1	A	174	ILE	2.2
10	W	35	PHE	2.2
8	H	71	HIS	2.2
2	B	34	ILE	2.2
3	P	96	PHE	2.2
5	E	182	VAL	2.2
2	B	206	LEU	2.2
1	A	1	ALA	2.2
2	B	132	PHE	2.2
7	G	81	GLN	2.2
1	N	269	VAL	2.2
3	P	90	PHE	2.2
8	U	12	GLU	2.2
8	U	78	LYS	2.2
9	I	49	LEU	2.1
3	P	2	ALA	2.1
4	Q	145	GLU	2.1
9	V	52	ARG	2.1
10	J	62	SER	2.1
2	O	140	LEU	2.1
5	E	137	GLY	2.1
3	P	37	LEU	2.1
1	A	127	ILE	2.1
2	O	146	VAL	2.1
9	I	58	ARG	2.1
2	O	85	ILE	2.1
1	N	380	GLY	2.1
1	N	72	CYS	2.1
2	O	295	LEU	2.1
7	T	74	PRO	2.1
2	B	191	LEU	2.0
3	C	240	PHE	2.1
9	V	59	SER	2.0
5	E	110	ALA	2.0
2	O	35	ILE	2.0
5	R	115	SER	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	194	THR	2.0
8	U	61	PHE	2.0
9	V	70	LEU	2.0
3	P	333	LEU	2.0
4	Q	241	LYS	2.0
5	E	128	LYS	2.0
5	R	156	TYR	2.0
3	P	234	THR	2.0
3	P	240	PHE	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
15	GOL	P	3011	6/6	0.88	0.45	7.31	84,86,87,88	0
11	PEE	A	2005	50/51	0.85	0.55	6.55	79,96,106,107	0
14	UQ	P	3002	19/63	0.75	0.54	5.94	126,136,137,137	0
14	UQ	C	2002	19/63	0.86	0.47	5.26	91,92,94,95	0
11	PEE	C	2007	49/51	0.95	0.41	4.48	46,67,84,85	0
11	PEE	P	3007	49/51	0.90	0.59	3.85	74,88,100,101	0
11	PEE	P	3005	50/51	0.80	0.54	3.55	92,105,114,115	0
11	PEE	A	2008	21/51	0.72	0.31	3.33	132,136,139,140	0
18	BOG	Q	3009	20/20	0.83	0.40	1.78	74,89,91,93	0
17	CDL	D	2003	42/100	0.89	0.27	1.72	92,101,111,114	0
12	HEM	P	501	43/43	0.98	0.32	1.47	42,49,60,64	0
12	HEM	C	502	43/43	0.98	0.31	1.38	32,37,47,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
13	AZO	C	2001	30/30	0.96	0.26	1.36	36,39,41,41	0
17	CDL	G	2004	40/100	0.93	0.28	1.12	73,85,100,101	0
17	CDL	Q	3003	42/100	0.85	0.27	1.08	117,129,145,145	0
18	BOG	P	2010	12/20	0.57	0.25	0.96	140,143,144,145	0
18	BOG	D	2009	20/20	0.91	0.28	0.94	60,72,75,76	0
12	HEM	C	501	43/43	0.98	0.29	0.91	35,40,50,55	0
15	GOL	C	2011	6/6	0.91	0.22	0.68	80,84,85,86	0
13	AZO	P	3001	30/30	0.95	0.26	0.54	52,60,66,67	0
16	HEC	Q	501	43/43	0.96	0.23	0.35	60,65,71,72	0
12	HEM	P	502	43/43	0.98	0.26	0.19	38,47,58,60	0
16	HEC	D	501	43/43	0.98	0.22	0.11	31,37,45,48	0
17	CDL	T	3004	40/100	0.91	0.22	-0.01	97,104,113,114	0
19	FES	R	501	4/4	0.99	0.14	-0.85	88,89,90,91	0
19	FES	E	501	4/4	0.95	0.13	-1.73	153,153,154,154	0
18	BOG	D	2091	13/20	0.41	0.33	-	207,208,208,208	0
18	BOG	Q	3091	13/20	0.16	0.44	-	192,194,195,195	0
11	PEE	N	3008	5/51	0.85	0.21	-	110,111,112,112	0

6.5 Other polymers ⓘ

There are no such residues in this entry.