Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:04 AM GMT

PDB ID	:	3CXH
Title	:	Structure of yeast complex III with isoform-2 cytochrome c bound and definition of a minimal core interface for electron transfer.
Authors	:	Solmaz, S.R.N.; Hunte, C.
Deposited on	:	2008-04-24
Resolution	:	2.50 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 ①) were used in the production of this report:

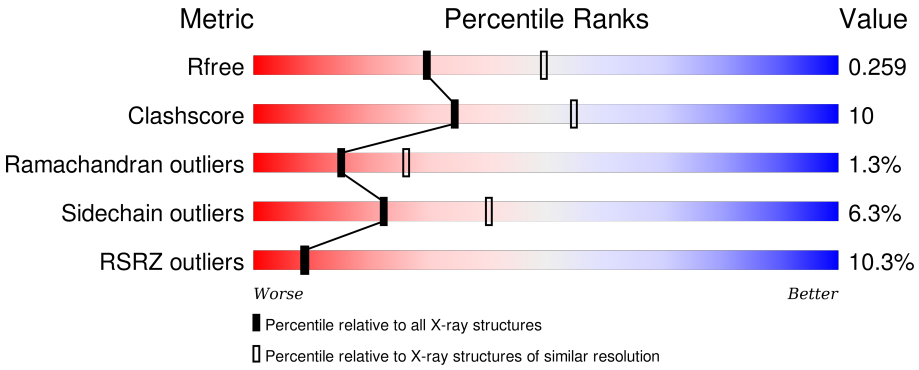
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	431	9% 68% 27% 5%
1	L	431	10% 75% 21% •
2	B	352	9% 69% 26% •
2	M	352	9% 69% 26% 5%
3	C	385	2% 80% 18% •

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Mol	Chain	Length	Quality of chain
3	N	385	2% 86% 13%
4	D	248	4% 85% 12%
4	O	248	2% 83% 15%
5	E	185	11% 77% 21%
5	P	185	10% 81% 17%
6	F	146	9% 41% 8% 49%
6	Q	146	8% 40% 10% 49%
7	G	126	3% 79% 17%
7	R	126	5% 80% 17%
8	H	93	22% 80% 17%
8	S	93	25% 80% 20%
9	I	65	12% 77% 6% 15%
9	T	65	12% 71% 9% 5% 15%
10	J	127	16% 69% 28%
10	U	127	17% 66% 28% 6%
11	K	107	45% 56% 37% 7%
11	V	107	39% 71% 27%
12	W	112	21% 80% 17%

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
13	SUC	O	4146	-	-	-	X
19	9PE	C	4111	-	-	-	X
19	9PE	N	4011	-	-	-	X

2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 36805 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cytochrome b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	431	Total	C	N	O	S	0	0	0
			3344	2109	576	653	6			
1	L	431	Total	C	N	O	S	0	0	0
			3344	2109	576	653	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	153	ASP	GLU	CONFLICT	UNP P07256
L	153	ASP	GLU	CONFLICT	UNP P07256

- Molecule 2 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	352	Total	C	N	O	S	0	0	0
			2735	1747	453	534	1			
2	M	352	Total	C	N	O	S	0	0	0
			2735	1747	453	534	1			

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	385	Total	C	N	O	S	0	0	0
			3090	2082	484	503	21			
3	N	385	Total	C	N	O	S	0	0	0
			3090	2082	484	503	21			

- Molecule 4 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	246	Total	C	N	O	S	0	0	0
			1940	1237	334	360	9			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	O	246	Total	C	N	O	S	0	0	0
			1940	1237	334	360	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	185	Total	C	N	O	S	0	0	0
			1411	893	242	266	10			
5	P	185	Total	C	N	O	S	0	0	0
			1411	893	242	266	10			

- Molecule 6 is a protein called Cytochrome b-c1 complex subunit 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	74	Total	C	N	O	S	0	0	0
			624	391	108	123	2			
6	Q	74	Total	C	N	O	S	0	0	0
			624	391	108	123	2			

- Molecule 7 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	125	Total	C	N	O	S	0	0	0
			1012	648	172	190	2			
7	R	125	Total	C	N	O	S	0	0	0
			1012	648	172	190	2			

- Molecule 8 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	93	Total	C	N	O	S	0	0	0
			773	510	131	130	2			
8	S	93	Total	C	N	O	S	0	0	0
			773	510	131	130	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	I	55	Total	C	N	O	0	0	0
			448	298	75	75			
9	T	55	Total	C	N	O	0	0	0
			448	298	75	75			

- Molecule 10 is a protein called HEAVY CHAIN (VH) OF FV-FRAGMENT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	127	Total	C	N	O	S	0	0	0
			1015	644	167	201	3			
10	U	127	Total	C	N	O	S	0	0	0
			1015	644	167	201	3			

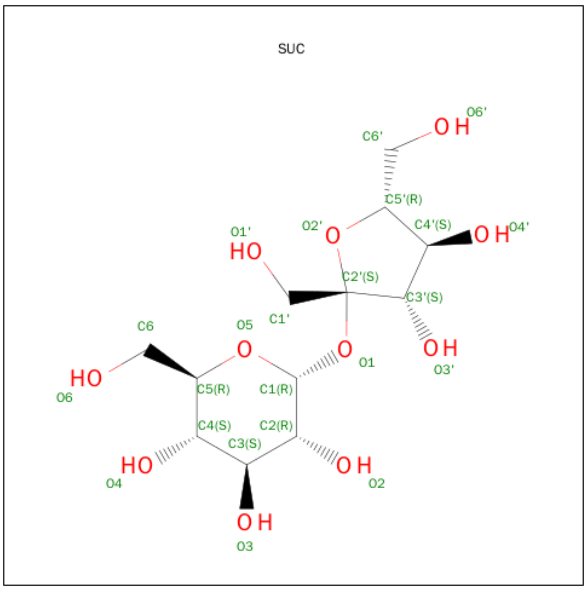
- Molecule 11 is a protein called LIGHT CHAIN (VL) OF FV-FRAGMENT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	107	Total	C	N	O	S	0	0	0
			842	536	141	163	2			
11	V	107	Total	C	N	O	S	0	0	0
			842	536	141	163	2			

- Molecule 12 is a protein called Cytochrome c iso-2.

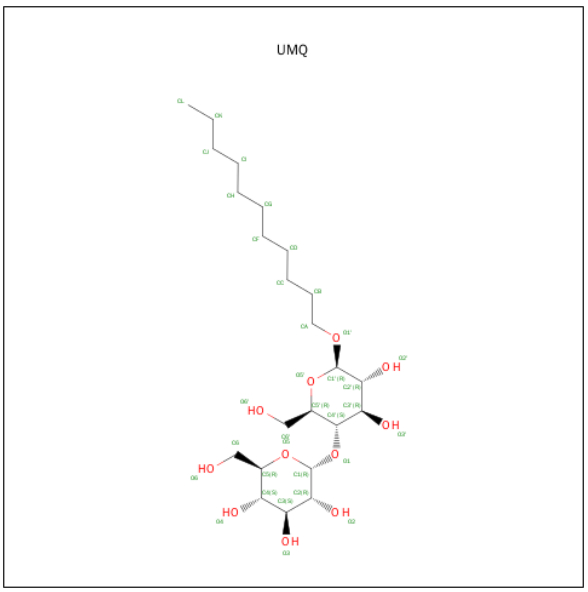
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	W	112	Total	C	N	O	S	0	1	0
			885	555	159	166	5			

- Molecule 13 is SUGAR (SUCROSE) (three-letter code: SUC) (formula: $C_{12}H_{22}O_{11}$).



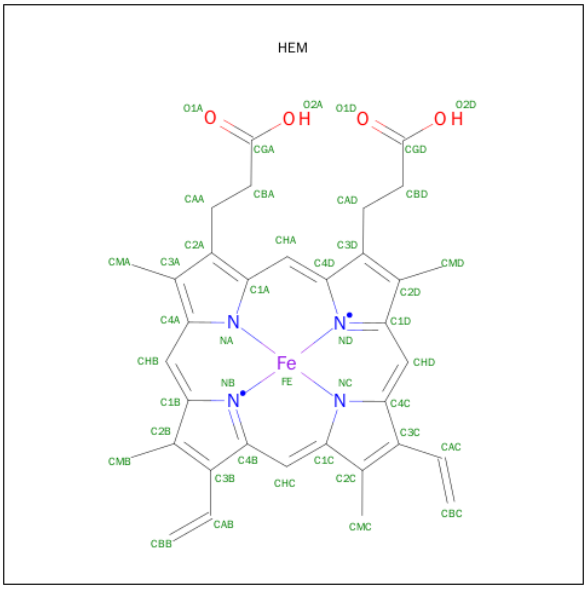
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	O	1	Total	C	O	0	0
			23	12	11		

- Molecule 14 is UNDECYL-MALTOSIDE (three-letter code: UMQ) (formula: $C_{23}H_{44}O_{11}$).



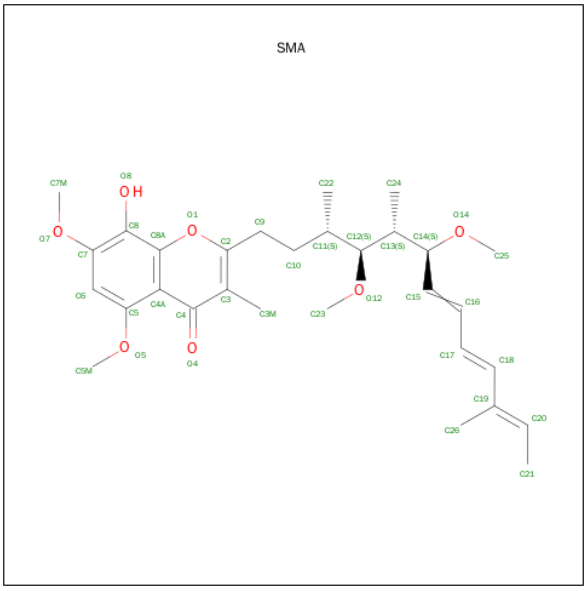
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	A	1	Total C O 34 23 11	0	0
14	L	1	Total C O 34 23 11	0	0

- Molecule 15 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



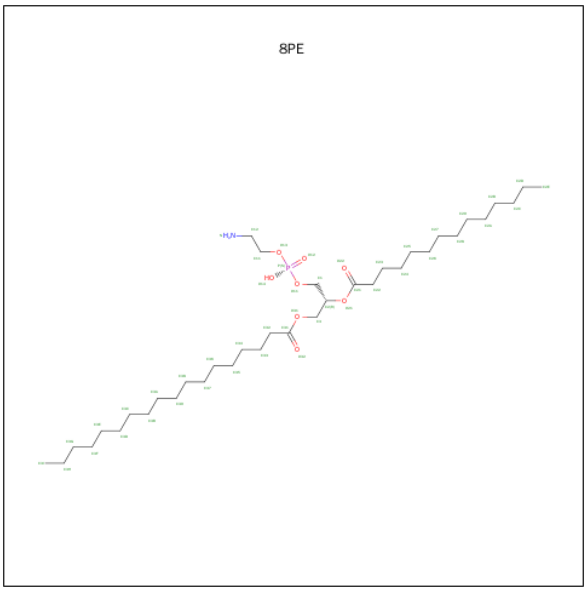
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
15	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
15	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
15	N	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
15	N	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
15	O	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4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

- Molecule 16 is STIGMATELLIN A (three-letter code: SMA) (formula: $C_{30}H_{42}O_7$).



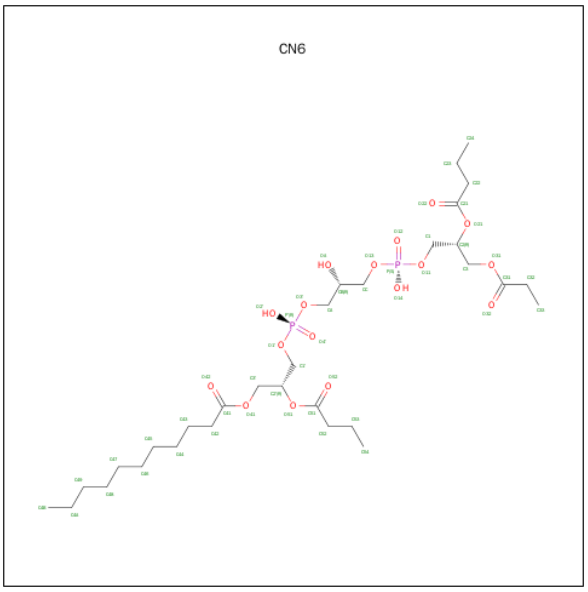
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	C	1	Total	C	O	0	0
			37	30	7		
16	N	1	Total	C	O	0	0
			37	30	7		

- Molecule 17 is (2R)-3-{[(S)-(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-2-(TETRADECANOYLOXY)PROPYL OCTADECANOATE (three-letter code: 8PE) (formula: $C_{37}H_{74}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	C	1	Total	C	N	O	P	0	0
			47	37	1	8	1		
17	N	1	Total	C	N	O	P	0	0
			47	37	1	8	1		

- Molecule 18 is (2R,5R,11S,14R)-2-(BUTANOYLOXY)-5,8,11-TRIHYDROXY-5,11-DIOXIDO-16-OXO-14-[(PROPANOYLOXY)METHYL]-4,6,10,12,15-PENTAOXA-5,11-DIPHOSPHANONADEC-1-YL UNDECANOATE (three-letter code: CN6) (formula: $C_{31}H_{58}O_{17}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	C	1	Total	C	O	P	0	0
			50	31	17	2		

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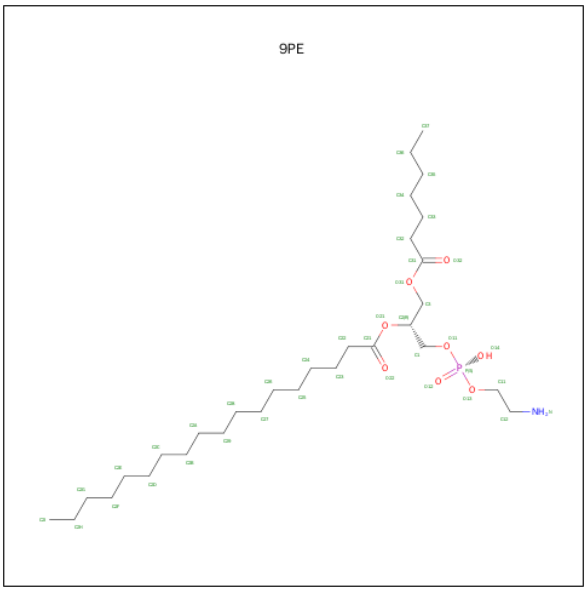
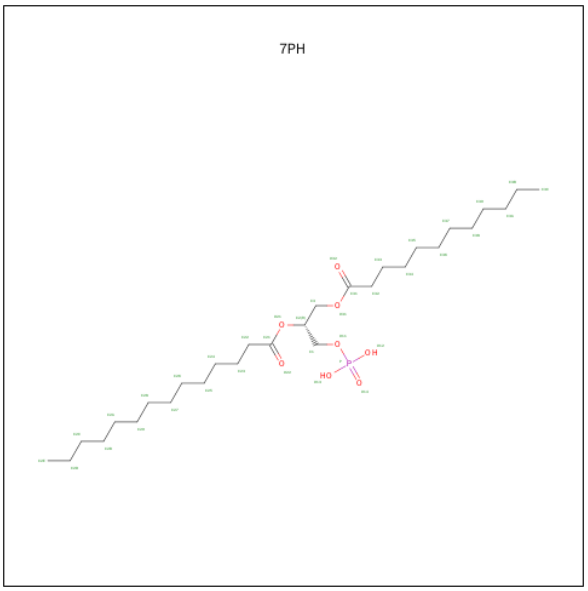
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	N	1	Total	C	O	P	0	0
			50	31	17	2		

- Molecule 19 is (1R)-2-{[(S)-(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(HEPTANOYLOXY)METHYL]ETHYL OCTADECANOATE (three-letter code: 9PE) (formula: $C_{30}H_{60}NO_8P$).



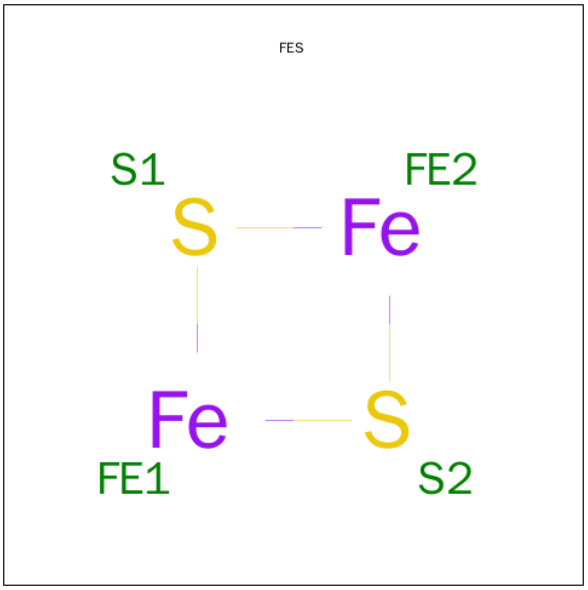
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	C	1	Total	C	N	O	P	0	0
			40	30	1	8	1		
19	N	1	Total	C	N	O	P	0	0
			40	30	1	8	1		

- Molecule 20 is (1R)-2-(DODECANOYLOXY)-1-[(PHOSPHONOOXY)METHYL]ETHYL TETRADECANOATE (three-letter code: 7PH) (formula: $C_{29}H_{57}O_8P$).



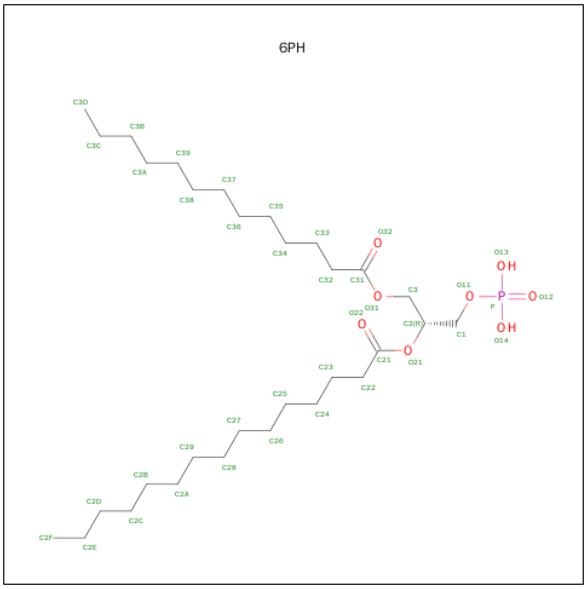
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	D	1	Total	C	O	P	0	0
			38	29	8	1		
20	O	1	Total	C	O	P	0	0
			38	29	8	1		

- Molecule 21 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	E	1	Total	Fe	S	0	0
			4	2	2		
21	P	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 22 is (1R)-2-(PHOSPHONOOXY)-1-[(TRIDECANOYLOXY)METHYL]ETHYL PENTADECANOATE (three-letter code: 6PH) (formula: $C_{31}H_{61}O_8P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	E	1	Total C O P 40 31 8 1	0	0
22	L	1	Total C O P 40 31 8 1	0	0

- Molecule 23 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	A	42	Total O 42 42	0	0
23	B	17	Total O 17 17	0	0
23	C	75	Total O 75 75	0	0
23	D	50	Total O 50 50	0	0
23	E	19	Total O 19 19	0	0
23	F	3	Total O 3 3	0	0
23	G	21	Total O 21 21	0	0
23	H	10	Total O 10 10	0	0

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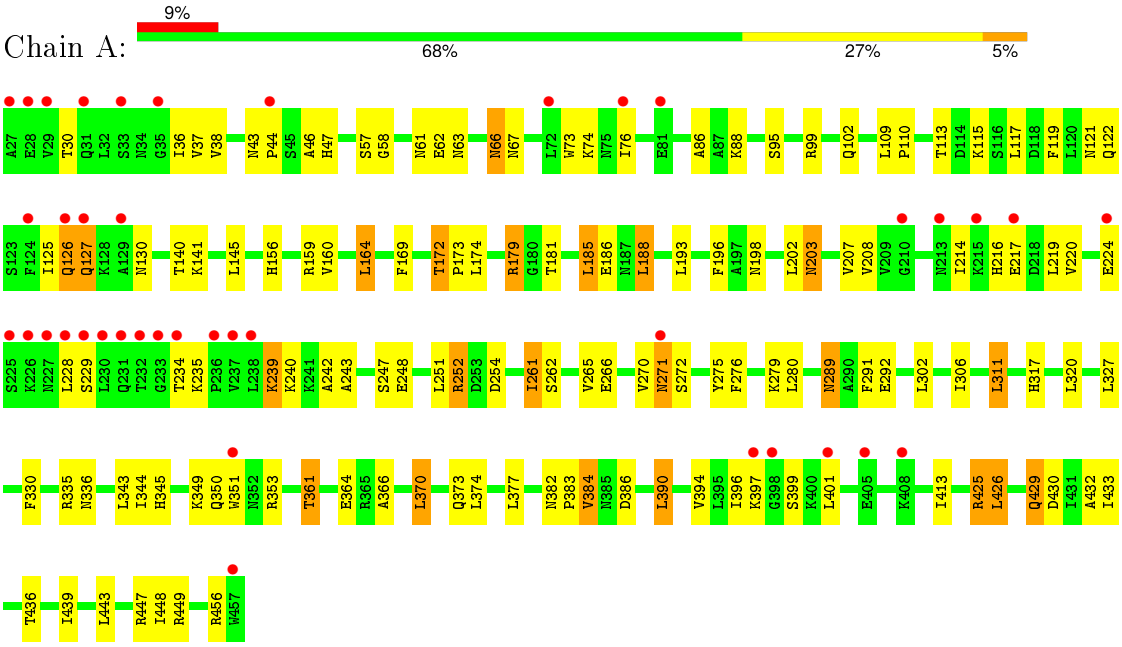
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	I	4	Total O 4 4	0	0
23	J	2	Total O 2 2	0	0
23	K	1	Total O 1 1	0	0
23	L	54	Total O 54 54	0	0
23	M	15	Total O 15 15	0	0
23	N	88	Total O 88 88	0	0
23	O	74	Total O 74 74	0	0
23	P	18	Total O 18 18	0	0
23	Q	3	Total O 3 3	0	0
23	R	22	Total O 22 22	0	0
23	S	13	Total O 13 13	0	0
23	T	5	Total O 5 5	0	0
23	U	2	Total O 2 2	0	0
23	W	10	Total O 10 10	0	0

3 Residue-property plots (i)

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

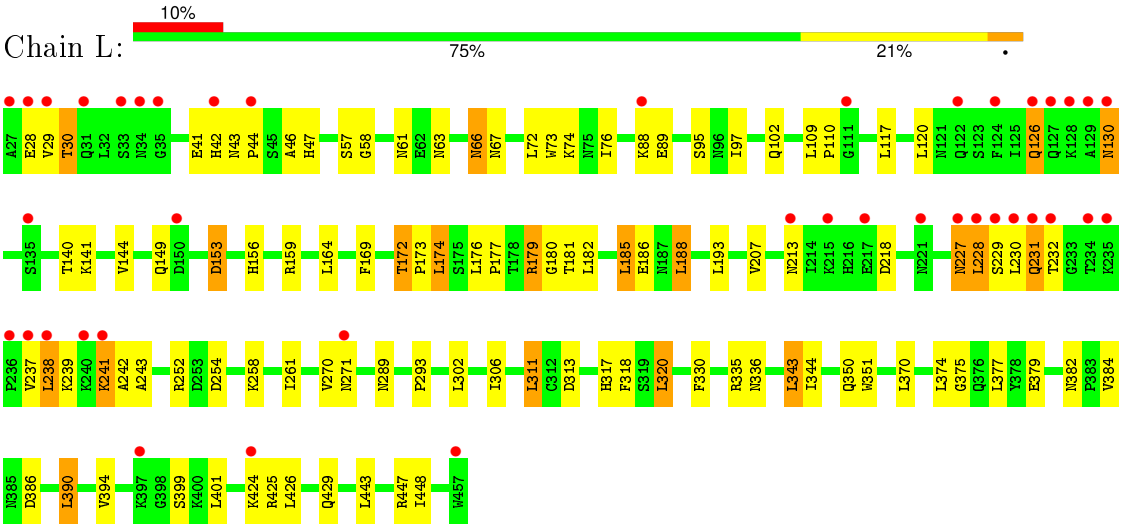
- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain A:



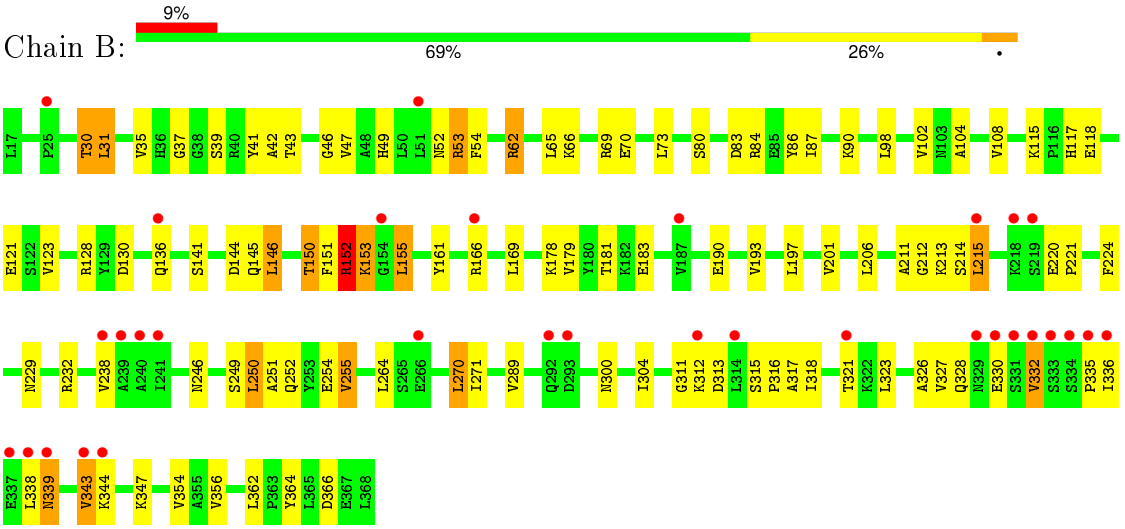
- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain L:



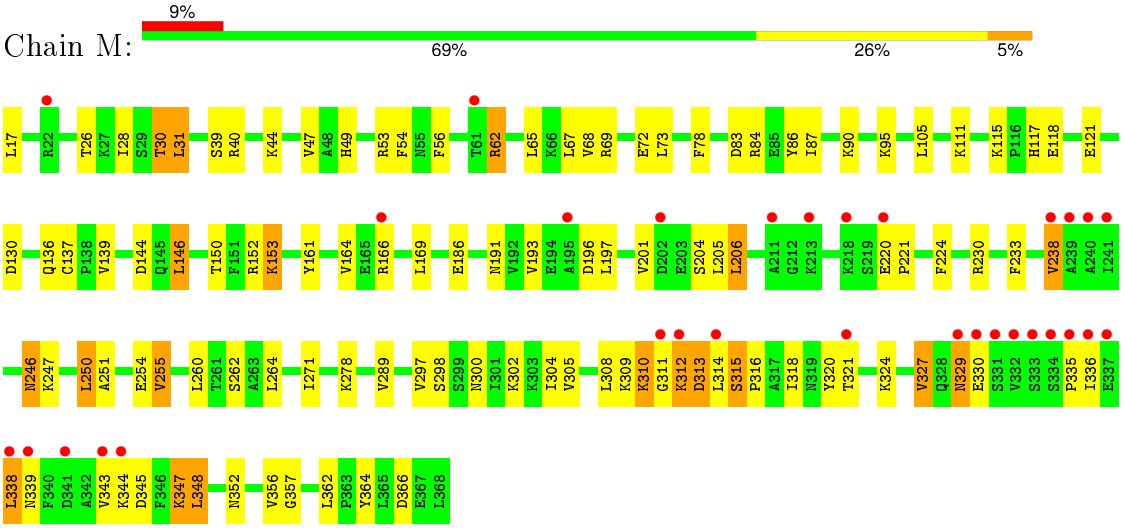
- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain B:



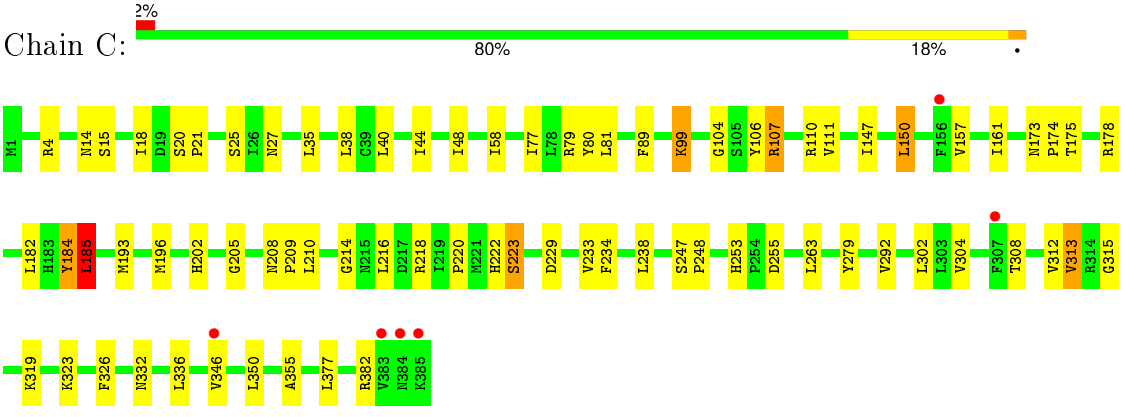
- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain M:



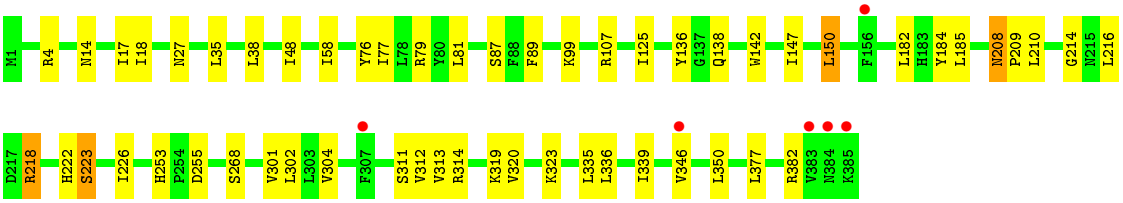
- Molecule 3: Cytochrome b

Chain C:

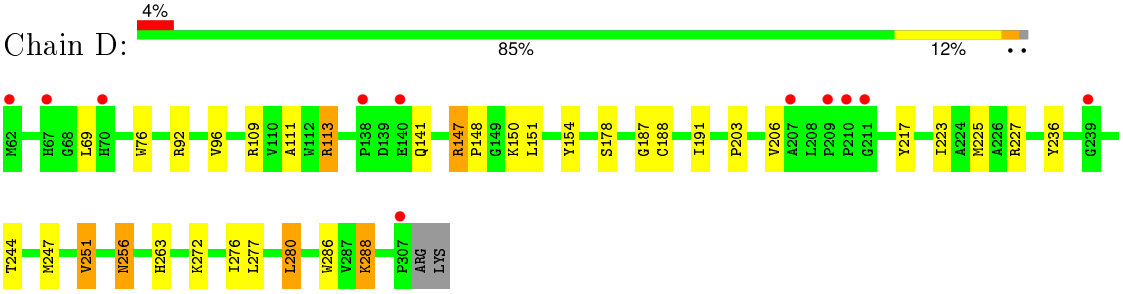


- Molecule 3: Cytochrome b

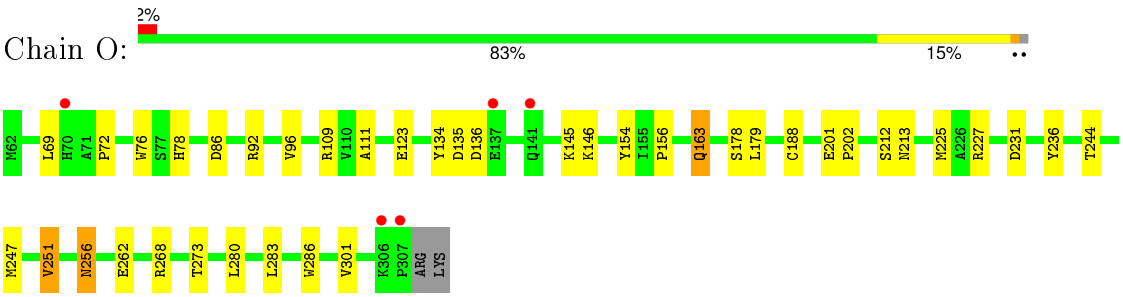
Chain N:



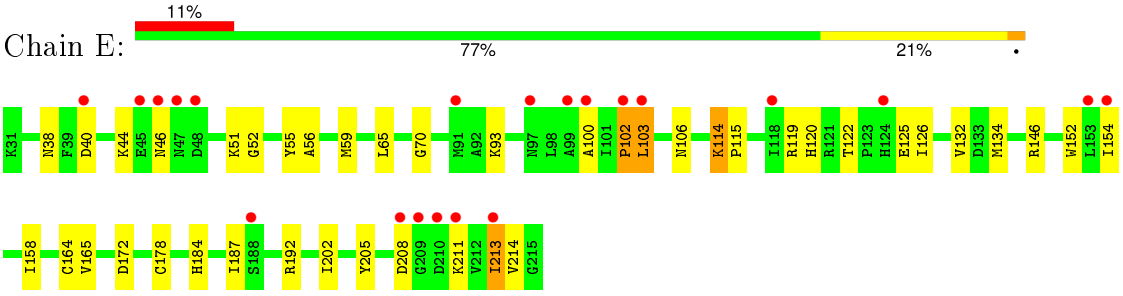
• Molecule 4: Cytochrome c1, heme protein, mitochondrial



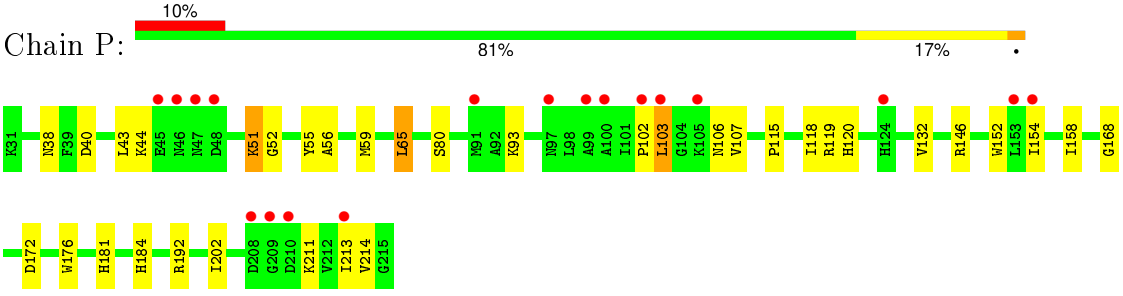
• Molecule 4: Cytochrome c1, heme protein, mitochondrial



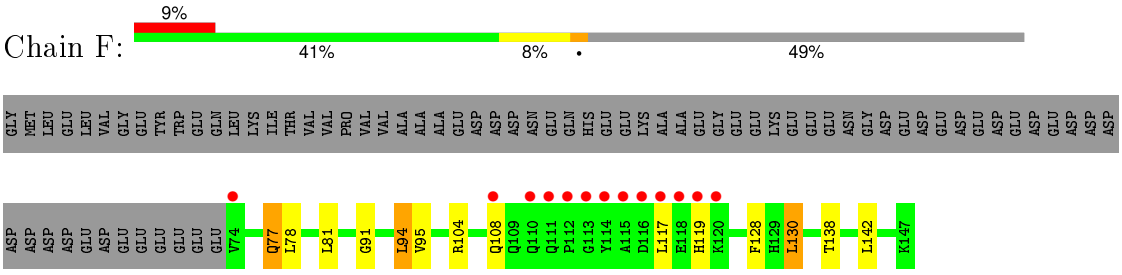
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial



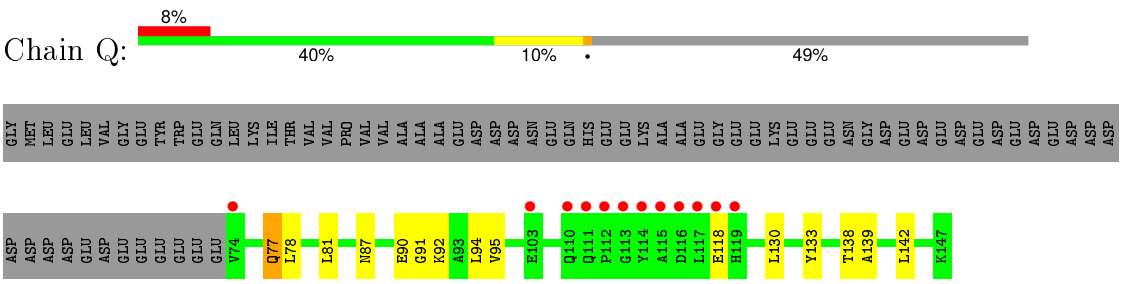
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial



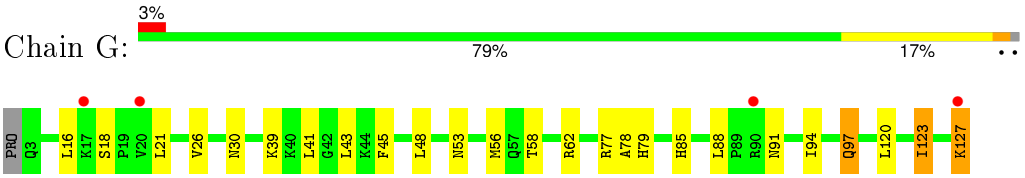
• Molecule 6: Cytochrome b-c1 complex subunit 6



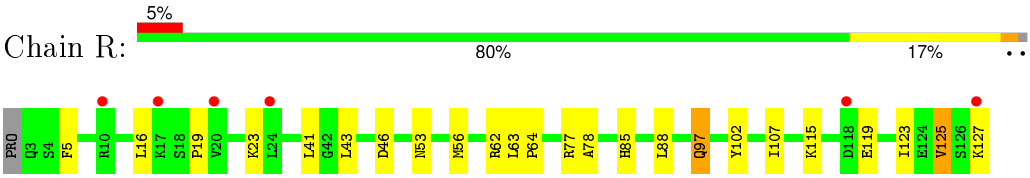
• Molecule 6: Cytochrome b-c1 complex subunit 6



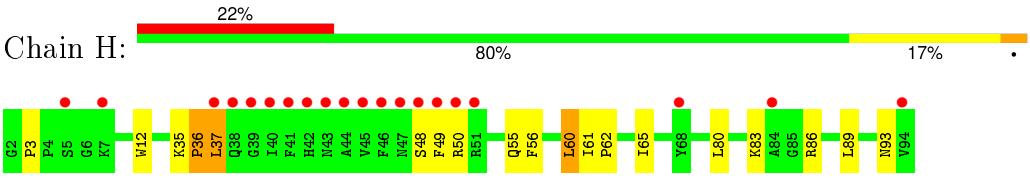
• Molecule 7: Cytochrome b-c1 complex subunit 7



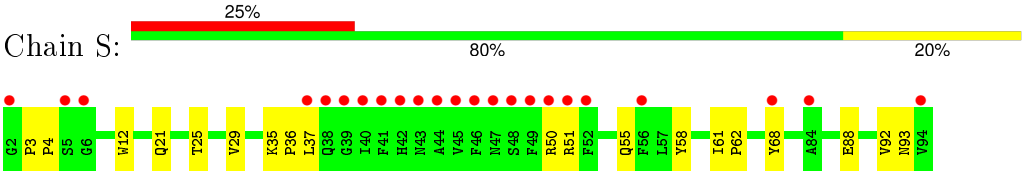
• Molecule 7: Cytochrome b-c1 complex subunit 7



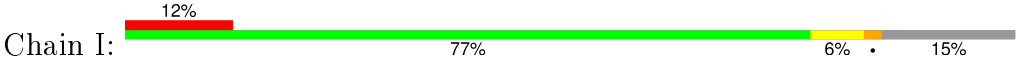
• Molecule 8: Cytochrome b-c1 complex subunit 8

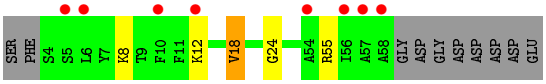


• Molecule 8: Cytochrome b-c1 complex subunit 8

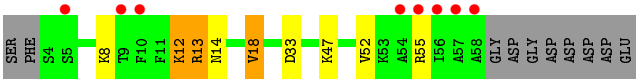


• Molecule 9: Cytochrome b-c1 complex subunit 9

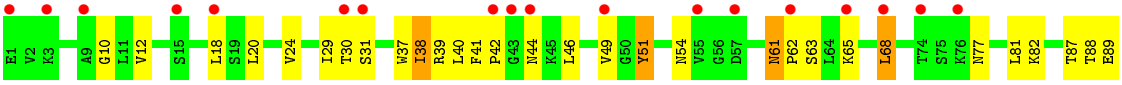


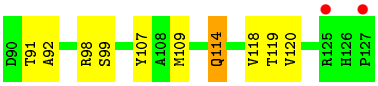


• Molecule 9: Cytochrome b-c1 complex subunit 9

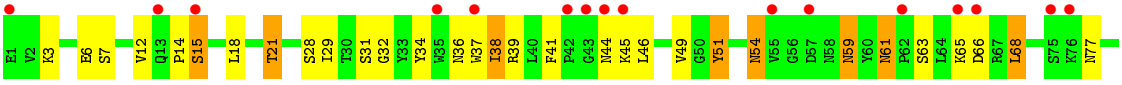


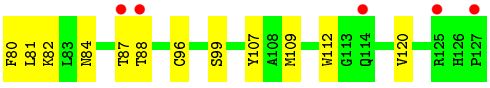
• Molecule 10: HEAVY CHAIN (VH) OF FV-FRAGMENT



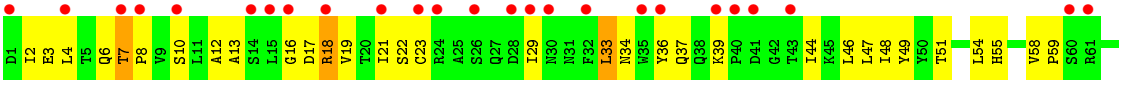


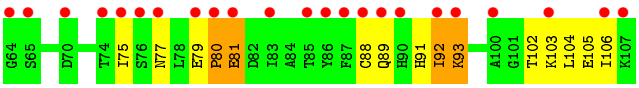
• Molecule 10: HEAVY CHAIN (VH) OF FV-FRAGMENT



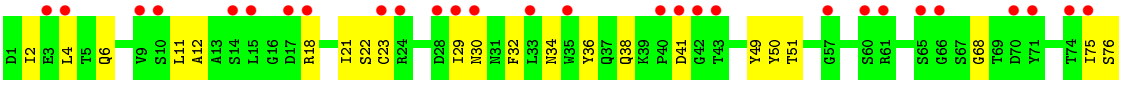


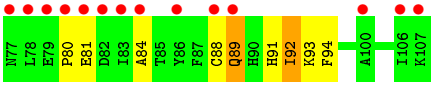
• Molecule 11: LIGHT CHAIN (VL) OF FV-FRAGMENT



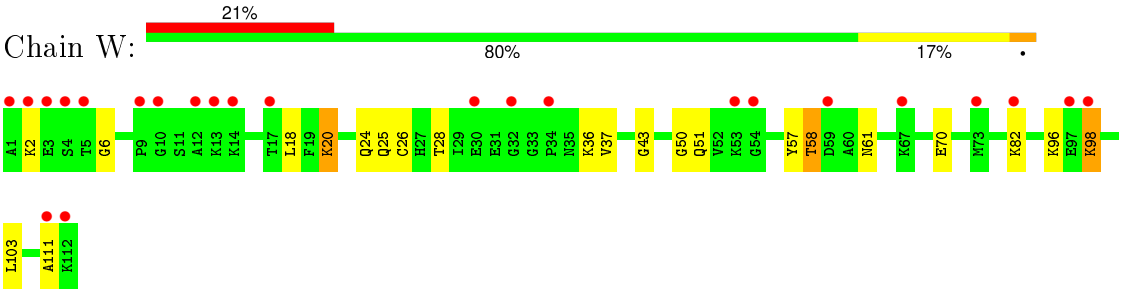


• Molecule 11: LIGHT CHAIN (VL) OF FV-FRAGMENT





• Molecule 12: Cytochrome c iso-2



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	145.54Å 162.97Å 194.23Å 90.00° 104.39° 90.00°	Depositor
Resolution (Å)	19.97 – 2.50 19.97 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.9 (19.97-2.50) 96.0 (19.97-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.66	Depositor
$< I/\sigma(I) >$ [1]	2.01 (at 2.50Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.225 , 0.256 0.227 , 0.259	Depositor DCC
R_{free} test set	14494 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	45.8	Xtriage
Anisotropy	0.430	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 56.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 289897 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	36805	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.27% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CN6, UMQ, 8PE, M3L, 7PH, FES, SUC, 9PE, HEM, 6PH, SMA

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	0.36	0/3405	0.61	1/4614 (0.0%)
1	L	0.37	0/3405	0.63	0/4614
2	B	0.36	0/2781	0.66	2/3764 (0.1%)
2	M	0.37	0/2781	0.65	1/3764 (0.0%)
3	C	0.43	0/3192	0.64	1/4354 (0.0%)
3	N	0.44	0/3192	0.66	0/4354
4	D	0.37	0/2001	0.61	0/2726
4	O	0.40	0/2001	0.63	0/2726
5	E	0.36	0/1444	0.60	0/1957
5	P	0.35	0/1444	0.61	1/1957 (0.1%)
6	F	0.36	0/638	0.53	0/858
6	Q	0.37	0/638	0.58	0/858
7	G	0.37	0/1032	0.62	0/1397
7	R	0.40	0/1032	0.63	0/1397
8	H	0.41	0/804	0.55	0/1088
8	S	0.44	0/804	0.56	0/1088
9	I	0.39	0/461	0.52	0/622
9	T	0.42	0/461	0.51	0/622
10	J	0.35	0/1043	0.60	0/1422
10	U	0.34	0/1043	0.62	0/1422
11	K	0.33	0/863	0.54	0/1172
11	V	0.33	0/863	0.53	0/1172
12	W	0.34	0/891	0.60	0/1191
All	All	0.38	0/36219	0.62	6/49139 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	P	65	LEU	CA-CB-CG	6.40	130.03	115.30
2	B	87	ILE	N-CA-C	-6.16	94.38	111.00
2	B	152	ARG	N-CA-C	5.45	125.71	111.00
2	M	87	ILE	N-CA-C	-5.44	96.31	111.00
1	A	251	LEU	CA-CB-CG	5.32	127.54	115.30
3	C	185	LEU	CA-CB-CG	5.15	127.15	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	279	TYR	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3344	0	3321	99	0
1	L	3344	0	3321	80	0
2	B	2735	0	2774	74	0
2	M	2735	0	2774	77	0
3	C	3090	0	3129	52	0
3	N	3090	0	3129	30	0
4	D	1940	0	1862	30	0
4	O	1940	0	1862	30	0
5	E	1411	0	1386	36	0
5	P	1411	0	1386	25	0
6	F	624	0	581	10	0
6	Q	624	0	581	9	0
7	G	1012	0	1026	22	0
7	R	1012	0	1026	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	H	773	0	736	14	0
8	S	773	0	736	15	0
9	I	448	0	445	5	0
9	T	448	0	445	7	0
10	J	1015	0	959	29	0
10	U	1015	0	959	35	0
11	K	842	0	820	33	0
11	V	842	0	820	23	0
12	W	885	0	890	15	0
13	O	23	0	22	2	0
14	A	34	0	44	4	0
14	L	34	0	44	2	0
15	C	86	0	60	3	0
15	D	43	0	30	0	0
15	N	86	0	60	1	0
15	O	43	0	30	1	0
15	W	43	0	30	2	0
16	C	37	0	42	1	0
16	N	37	0	42	1	0
17	C	47	0	73	2	0
17	N	47	0	73	2	0
18	C	50	0	56	7	0
18	N	50	0	56	5	0
19	C	40	0	59	0	0
19	N	40	0	59	0	0
20	D	38	0	55	3	0
20	O	38	0	55	2	0
21	E	4	0	0	0	0
21	P	4	0	0	1	0
22	E	40	0	59	1	0
22	L	40	0	59	0	0
23	A	42	0	0	0	0
23	B	17	0	0	1	0
23	C	75	0	0	4	0
23	D	50	0	0	0	0
23	E	19	0	0	0	0
23	F	3	0	0	0	0
23	G	21	0	0	1	0
23	H	10	0	0	0	0
23	I	4	0	0	0	0
23	J	2	0	0	1	0
23	K	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	L	54	0	0	2	0
23	M	15	0	0	0	0
23	N	88	0	0	3	0
23	O	74	0	0	2	0
23	P	18	0	0	0	0
23	Q	3	0	0	0	0
23	R	22	0	0	1	0
23	S	13	0	0	0	0
23	T	5	0	0	0	0
23	U	2	0	0	0	0
23	W	10	0	0	1	0
All	All	36805	0	35976	721	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 10.

All (721) 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)
2:M:347:LYS:H	2:M:347:LYS:HD3	1.19	1.01
1:A:63:ASN:H	1:A:66:ASN:HD21	1.06	1.00
1:A:382:ASN:HD21	1:A:384:VAL:HG22	1.22	0.99
1:L:63:ASN:H	1:L:66:ASN:ND2	1.60	0.99
6:Q:77:GLN:H	6:Q:77:GLN:HE21	1.08	0.98
6:F:77:GLN:H	6:F:77:GLN:HE21	0.96	0.93
11:V:75:ILE:HG22	11:V:76:SER:H	1.35	0.90
1:L:63:ASN:H	1:L:66:ASN:HD21	0.94	0.90
6:F:77:GLN:H	6:F:77:GLN:NE2	1.69	0.90
6:F:78:LEU:HD13	6:F:142:LEU:HD22	1.52	0.89
6:Q:77:GLN:H	6:Q:77:GLN:NE2	1.73	0.86
1:A:58:GLY:H	1:A:61:ASN:HD22	1.24	0.86
2:M:49:HIS:HD2	2:M:161:TYR:H	1.24	0.85
1:L:317:HIS:HE1	1:L:351:TRP:HE1	1.23	0.84
2:M:62:ARG:HG2	2:M:62:ARG:HH21	1.43	0.84
10:U:29:ILE:H	10:U:77:ASN:HD21	1.25	0.84
5:E:134:MET:HG3	10:J:31:SER:HB3	1.61	0.81
11:V:93:LYS:HZ3	11:V:94:PHE:H	1.29	0.81
2:M:150:THR:HG22	2:M:352:ASN:HD22	1.45	0.81
11:K:21:ILE:HG22	11:K:22:SER:H	1.47	0.78
6:F:77:GLN:HE21	6:F:77:GLN:N	1.78	0.78
2:B:181:THR:HB	2:B:212:GLY:H	1.47	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:29:ILE:HG12	10:J:77:ASN:ND2	1.99	0.77
2:M:246:ASN:HD22	2:M:246:ASN:H	1.32	0.77
1:A:429:GLN:HA	1:A:429:GLN:HE21	1.48	0.76
1:L:179:ARG:HH21	1:L:179:ARG:HG2	1.49	0.76
2:M:347:LYS:N	2:M:347:LYS:HD3	1.98	0.75
10:J:99:SER:HB3	10:J:109:MET:HG2	1.69	0.75
7:G:77:ARG:HD3	7:G:88:LEU:HD11	1.67	0.75
2:B:49:HIS:HD2	2:B:161:TYR:H	1.34	0.75
1:L:344:ILE:HG21	1:L:448:ILE:HD12	1.68	0.75
2:B:62:ARG:HG2	2:B:62:ARG:HH21	1.50	0.75
2:M:49:HIS:CD2	2:M:161:TYR:H	2.05	0.75
5:E:44:LYS:NZ	5:E:52:GLY:H	1.83	0.75
9:T:8:LYS:O	9:T:12:LYS:HG3	1.87	0.75
11:V:6:GLN:HG2	11:V:23:CYS:SG	2.27	0.74
2:M:150:THR:HG22	2:M:352:ASN:ND2	2.03	0.74
4:D:286:TRP:CE3	5:E:59:MET:HG3	2.23	0.74
7:R:77:ARG:HD3	7:R:88:LEU:HD11	1.69	0.74
1:L:63:ASN:N	1:L:66:ASN:HD21	1.79	0.74
2:M:238:VAL:HG13	2:M:356:VAL:HB	1.68	0.74
4:O:96:VAL:HB	4:O:251:VAL:HG13	1.69	0.73
1:L:58:GLY:H	1:L:61:ASN:HD22	1.37	0.73
3:N:208:ASN:HD22	3:N:210:LEU:H	1.36	0.73
1:A:73:TRP:CE3	1:A:76:ILE:HD11	2.24	0.73
2:B:336:ILE:HD12	2:B:336:ILE:H	1.54	0.73
2:B:238:VAL:HG13	2:B:356:VAL:HB	1.71	0.72
1:A:382:ASN:ND2	1:A:384:VAL:HG22	2.01	0.72
2:B:300:ASN:O	2:B:304:ILE:HG12	1.89	0.72
3:C:208:ASN:HD22	3:C:210:LEU:H	1.38	0.72
1:A:317:HIS:HE1	1:A:351:TRP:HE1	1.38	0.72
1:A:63:ASN:H	1:A:66:ASN:ND2	1.83	0.71
5:E:172:ASP:H	5:E:184:HIS:HD2	1.38	0.71
17:N:4110:8PE:H1A	8:S:51:ARG:HE	1.56	0.71
4:D:272:LYS:O	4:D:276:ILE:HG22	1.90	0.71
2:M:137:CYS:SG	2:M:139:VAL:HG22	2.31	0.71
2:M:324:LYS:O	2:M:327:VAL:HG22	1.90	0.71
1:L:317:HIS:CE1	1:L:351:TRP:HE1	2.06	0.70
2:M:347:LYS:HG2	2:M:348:LEU:H	1.55	0.70
18:C:4031:CN6:HAA	7:G:85:HIS:NE2	2.06	0.70
1:A:228:LEU:HG	1:A:229:SER:H	1.56	0.70
1:L:241:LYS:HD2	1:L:241:LYS:H	1.57	0.69
3:N:214:GLY:O	3:N:218:ARG:HD2	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:37:GLY:HA3	2:B:179:VAL:HG11	1.73	0.69
3:C:214:GLY:O	3:C:218:ARG:HD2	1.92	0.69
2:B:30:THR:HG23	2:B:190:GLU:HB3	1.74	0.69
1:A:66:ASN:H	1:A:66:ASN:HD22	1.41	0.69
11:K:29:ILE:HG22	11:K:92:ILE:HD12	1.74	0.69
11:K:47:LEU:HA	11:K:58:VAL:HG11	1.74	0.69
18:N:4131:CN6:HAA	7:R:85:HIS:NE2	2.08	0.68
18:N:4131:CN6:HC	23:N:6998:HOH:O	1.92	0.68
3:C:107:ARG:HH21	3:C:107:ARG:HG3	1.58	0.68
1:A:361:THR:HG21	7:R:123:ILE:O	1.94	0.68
10:J:114:GLN:H	10:J:114:GLN:NE2	1.92	0.68
5:P:44:LYS:NZ	5:P:52:GLY:H	1.91	0.68
11:K:36:TYR:HE2	11:K:89:GLN:HG2	1.59	0.67
1:A:217:GLU:HA	1:A:220:VAL:HG12	1.76	0.67
1:A:127:GLN:HG2	1:A:130:ASN:HD22	1.60	0.67
3:N:323:LYS:CE	8:S:55:GLN:HE22	2.08	0.67
1:L:130:ASN:HD22	1:L:130:ASN:N	1.92	0.66
10:J:61:ASN:HD22	10:J:63:SER:H	1.44	0.66
8:H:56:PHE:O	8:H:60:LEU:HB2	1.96	0.66
5:P:172:ASP:H	5:P:184:HIS:HD2	1.43	0.66
10:J:38:ILE:HD11	10:J:46:LEU:HD22	1.78	0.66
10:U:61:ASN:HD22	10:U:63:SER:H	1.42	0.66
2:M:300:ASN:O	2:M:304:ILE:HG12	1.96	0.65
23:O:6502:HOH:O	12:W:25:GLN:HG3	1.95	0.65
3:C:185:LEU:HG	3:N:48:ILE:HD13	1.79	0.65
5:P:132:VAL:HG21	5:P:192:ARG:NH1	2.11	0.65
1:A:66:ASN:HA	1:A:188:LEU:HD11	1.79	0.65
10:U:41:PHE:HB2	10:U:45:LYS:HG3	1.79	0.65
1:L:172:THR:HG23	1:L:242:ALA:HA	1.79	0.64
4:D:147:ARG:HH21	4:D:150:LYS:HE3	1.62	0.64
3:C:253:HIS:HD2	3:C:255:ASP:H	1.45	0.64
9:T:52:VAL:HA	9:T:55:ARG:HD3	1.77	0.64
2:B:152:ARG:HH12	2:M:366:ASP:HB2	1.62	0.63
1:L:156:HIS:HD2	1:L:159:ARG:HH21	1.45	0.63
6:Q:77:GLN:N	6:Q:77:GLN:HE21	1.88	0.63
1:L:270:VAL:O	1:L:271:ASN:HB2	1.97	0.63
1:L:228:LEU:HG	1:L:229:SER:H	1.63	0.63
4:O:227:ARG:HH11	4:O:244:THR:HG21	1.63	0.63
2:M:31:LEU:HD12	2:M:105:LEU:HD12	1.81	0.63
5:P:103:LEU:O	5:P:120:HIS:HB3	1.98	0.63
5:E:106:ASN:ND2	5:E:119:ARG:HB2	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:SER:O	1:A:102:GLN:HG3	1.99	0.62
3:N:323:LYS:NZ	8:S:55:GLN:HE22	1.98	0.62
3:C:27:ASN:HB2	18:C:4031:CN6:O2'	1.99	0.62
2:B:152:ARG:O	2:B:153:LYS:HB2	2.00	0.62
1:A:99:ARG:HD3	1:A:174:LEU:HD12	1.80	0.62
2:M:329:ASN:N	2:M:329:ASN:HD22	1.98	0.62
1:A:276:PHE:HZ	1:A:401:LEU:HD21	1.64	0.62
7:G:62:ARG:HD2	2:M:121:GLU:OE2	1.98	0.62
1:A:172:THR:HG23	1:A:242:ALA:HA	1.82	0.62
1:L:179:ARG:NH2	1:L:179:ARG:HG2	2.14	0.62
2:M:336:ILE:H	2:M:336:ILE:HD12	1.65	0.62
10:U:38:ILE:HD11	10:U:46:LEU:HD22	1.80	0.62
2:M:315:SER:N	2:M:316:PRO:HD3	2.15	0.62
2:M:83:ASP:HB2	2:M:86:TYR:H	1.65	0.61
3:N:253:HIS:HD2	3:N:255:ASP:H	1.48	0.61
4:D:96:VAL:HB	4:D:251:VAL:HG13	1.83	0.61
7:R:77:ARG:HD2	23:R:5803:HOH:O	1.99	0.61
11:K:21:ILE:HG22	11:K:22:SER:N	2.15	0.61
5:E:172:ASP:H	5:E:184:HIS:CD2	2.18	0.61
1:L:72:LEU:HD23	1:L:193:LEU:HD21	1.81	0.61
7:G:77:ARG:HD2	23:G:5303:HOH:O	2.00	0.61
4:O:213:ASN:OD1	13:O:4146:SUC:H6'2	2.00	0.61
10:U:68:LEU:HA	10:U:82:LYS:O	2.01	0.61
1:L:207:VAL:HG11	1:L:394:VAL:HG21	1.81	0.61
6:Q:78:LEU:HD13	6:Q:142:LEU:HD22	1.83	0.61
10:U:14:PRO:O	10:U:15:SER:HB3	2.01	0.61
3:C:44:ILE:O	3:C:48:ILE:HG12	2.01	0.60
1:L:149:GLN:O	1:L:153:ASP:HB2	2.02	0.60
2:B:152:ARG:HD3	2:B:224:PHE:CE1	2.36	0.60
7:G:43:LEU:HD21	7:G:78:ALA:CB	2.32	0.60
11:V:2:ILE:H	11:V:2:ILE:HD12	1.66	0.60
10:J:30:THR:O	10:J:54:ASN:HB2	2.00	0.60
3:N:253:HIS:CD2	3:N:255:ASP:H	2.19	0.60
14:A:4021:UMQ:HK1	22:E:4013:6PH:H39	1.83	0.60
11:V:34:ASN:ND2	11:V:50:TYR:H	1.99	0.60
2:M:65:LEU:O	2:M:69:ARG:HG2	2.00	0.60
3:C:4:ARG:HE	3:C:14:ASN:ND2	1.99	0.60
3:C:4:ARG:HE	3:C:14:ASN:HD21	1.50	0.60
1:L:229:SER:HB3	1:L:232:THR:HG21	1.84	0.60
10:U:41:PHE:HB2	10:U:45:LYS:CG	2.32	0.59
11:K:2:ILE:HD12	11:K:2:ILE:H	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:PHE:O	1:A:172:THR:HB	2.01	0.59
2:M:68:VAL:O	2:M:72:GLU:HG3	2.01	0.59
4:O:109:ARG:HG3	4:O:178:SER:CB	2.32	0.59
8:H:12:TRP:CE2	8:S:3:PRO:HG3	2.38	0.59
10:U:29:ILE:H	10:U:77:ASN:ND2	1.98	0.59
3:N:27:ASN:HB2	18:N:4131:CN6:O2'	2.02	0.59
4:O:78:HIS:HD2	23:O:5586:HOH:O	1.85	0.59
2:M:246:ASN:H	2:M:246:ASN:ND2	1.99	0.59
1:A:38:VAL:HA	1:A:208:VAL:HG13	1.85	0.59
5:E:93:LYS:HG3	5:E:214:VAL:O	2.02	0.59
10:U:28:SER:HB3	10:U:31:SER:OG	2.02	0.59
7:G:26:VAL:HG12	7:G:30:ASN:HD21	1.68	0.59
12:W:58:THR:HG22	12:W:61:ASN:H	1.68	0.59
1:L:394:VAL:HG12	1:L:399:SER:HA	1.85	0.59
1:A:117:LEU:HD11	1:A:219:LEU:HD12	1.84	0.58
4:D:247:MET:O	4:D:251:VAL:HG22	2.03	0.58
1:A:127:GLN:HG2	1:A:130:ASN:ND2	2.18	0.58
1:A:172:THR:HG23	1:A:173:PRO:HD2	1.85	0.58
4:O:201:GLU:HG3	4:O:202:PRO:HD2	1.86	0.58
2:M:308:LEU:HB2	2:M:348:LEU:HD22	1.85	0.58
1:L:382:ASN:OD1	1:L:384:VAL:HG22	2.03	0.58
5:E:115:PRO:HD2	5:E:158:ILE:HD11	1.84	0.58
11:V:75:ILE:HG22	11:V:76:SER:N	2.14	0.58
11:V:2:ILE:HD12	11:V:2:ILE:N	2.19	0.58
11:K:34:ASN:HD22	11:K:49:TYR:HA	1.67	0.58
3:N:208:ASN:HB2	3:N:209:PRO:HD2	1.86	0.58
3:N:147:ILE:O	3:N:150:LEU:HB2	2.03	0.58
5:P:51:LYS:HE2	5:P:55:TYR:CE1	2.39	0.58
3:C:40:LEU:HD12	15:C:4001:HEM:HBB1	1.86	0.58
1:A:252:ARG:HD3	1:A:254:ASP:OD1	2.04	0.58
14:L:4121:UMQ:O2'	9:T:18:VAL:HG22	2.04	0.58
2:B:49:HIS:CD2	2:B:161:TYR:H	2.19	0.57
2:M:146:LEU:O	2:M:150:THR:HG23	2.03	0.57
2:M:313:ASP:HB3	2:M:344:LYS:O	2.04	0.57
8:S:61:ILE:HB	8:S:62:PRO:HD3	1.85	0.57
1:A:234:THR:HG22	1:A:235:LYS:H	1.70	0.57
10:U:107:TYR:H	11:V:91:HIS:CD2	2.22	0.57
1:A:160:VAL:CG2	1:A:436:THR:HG22	2.35	0.57
3:C:173:ASN:HB3	3:C:174:PRO:HD3	1.85	0.57
8:H:12:TRP:CZ2	8:S:3:PRO:HG3	2.40	0.57
7:R:19:PRO:O	7:R:23:LYS:HG3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:24:VAL:HG21	10:J:29:ILE:HD11	1.85	0.56
1:L:172:THR:CG2	1:L:242:ALA:HA	2.35	0.56
11:V:36:TYR:HE2	11:V:89:GLN:HG2	1.69	0.56
5:E:103:LEU:O	5:E:120:HIS:HB3	2.05	0.56
5:P:172:ASP:H	5:P:184:HIS:CD2	2.23	0.56
6:F:81:LEU:HB3	6:F:138:THR:HG22	1.88	0.56
8:H:80:LEU:HB3	8:H:89:LEU:HD23	1.87	0.56
2:B:366:ASP:CB	2:M:152:ARG:HH12	2.19	0.56
5:E:44:LYS:HZ2	5:E:52:GLY:H	1.53	0.56
2:B:155:LEU:H	2:B:155:LEU:HD12	1.71	0.55
11:K:4:LEU:HD23	11:K:23:CYS:HB3	1.87	0.55
5:E:106:ASN:HD22	5:E:119:ARG:HB2	1.71	0.55
2:M:347:LYS:HG2	2:M:348:LEU:N	2.20	0.55
9:I:8:LYS:O	9:I:12:LYS:HD2	2.06	0.55
1:A:202:LEU:HD13	1:A:234:THR:HB	1.88	0.55
3:C:147:ILE:O	3:C:150:LEU:HB2	2.06	0.55
2:B:197:LEU:O	2:B:201:VAL:HG23	2.06	0.55
11:V:93:LYS:NZ	11:V:94:PHE:H	2.01	0.55
10:U:54:ASN:HD22	10:U:54:ASN:H	1.53	0.55
2:B:238:VAL:CG1	2:B:356:VAL:HB	2.36	0.55
10:J:61:ASN:ND2	10:J:63:SER:H	2.04	0.55
5:E:103:LEU:HG	5:E:122:THR:HG22	1.89	0.55
1:L:74:LYS:HG3	1:L:95:SER:HB3	1.89	0.55
5:P:55:TYR:O	5:P:59:MET:HG2	2.07	0.55
12:W:96:LYS:HD3	12:W:98:LYS:NZ	2.22	0.55
3:C:253:HIS:CD2	3:C:255:ASP:H	2.24	0.55
14:A:4021:UMQ:O2'	9:I:18:VAL:HG22	2.07	0.55
8:H:83:LYS:O	8:H:86:ARG:HG2	2.06	0.55
12:W:50:GLY:HA2	12:W:57:TYR:CE1	2.42	0.54
11:K:6:GLN:HG2	11:K:23:CYS:SG	2.47	0.54
5:P:118:ILE:HG12	5:P:154:ILE:HG12	1.89	0.54
1:A:46:ALA:O	1:A:47:HIS:HB2	2.07	0.54
20:D:4014:7PH:H35	5:E:70:GLY:HA3	1.88	0.54
3:C:304:VAL:HG12	3:C:308:THR:HG23	1.89	0.54
11:V:11:LEU:HG	11:V:12:ALA:H	1.72	0.54
1:L:29:VAL:HG12	1:L:30:THR:N	2.22	0.54
1:L:313:ASP:OD1	1:L:335:ARG:HD3	2.07	0.54
2:B:152:ARG:HG2	2:M:364:TYR:CE1	2.43	0.54
1:L:156:HIS:HD2	1:L:159:ARG:NH2	2.04	0.54
4:O:227:ARG:NH1	4:O:244:THR:HG21	2.22	0.54
1:L:46:ALA:O	1:L:47:HIS:HB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:V:38:GLN:O	11:V:84:ALA:HB1	2.07	0.54
10:J:40:LEU:O	10:J:92:ALA:HB1	2.07	0.54
2:B:151:PHE:O	2:B:153:LYS:N	2.37	0.54
2:M:152:ARG:HD3	2:M:224:PHE:CE1	2.43	0.54
1:L:241:LYS:CD	1:L:241:LYS:H	2.15	0.54
7:G:43:LEU:HD21	7:G:78:ALA:HB2	1.90	0.54
4:D:276:ILE:HD13	20:D:4014:7PH:O32	2.07	0.54
4:D:109:ARG:HG3	4:D:178:SER:CB	2.38	0.54
1:L:227:ASN:HD22	1:L:228:LEU:H	1.56	0.53
4:O:286:TRP:CE3	5:P:59:MET:HG3	2.43	0.53
1:A:289:ASN:HD22	1:A:289:ASN:C	2.11	0.53
1:A:207:VAL:HG11	1:A:394:VAL:HG21	1.90	0.53
10:J:61:ASN:HD22	10:J:62:PRO:N	2.05	0.53
1:L:258:LYS:HG2	1:L:335:ARG:HG3	1.91	0.53
2:M:115:LYS:HB2	2:M:118:GLU:HG3	1.89	0.53
3:C:14:ASN:ND2	3:C:18:ILE:HB	2.24	0.53
11:V:21:ILE:HG22	11:V:22:SER:N	2.24	0.53
2:M:197:LEU:O	2:M:201:VAL:HG23	2.09	0.53
1:A:67:ASN:ND2	1:A:181:THR:HG23	2.22	0.53
4:O:247:MET:O	4:O:251:VAL:HG22	2.09	0.53
1:A:317:HIS:CE1	1:A:351:TRP:HE1	2.24	0.53
18:N:4131:CN6:HAA	7:R:85:HIS:CE1	2.43	0.53
3:C:15:SER:O	3:C:202:HIS:HE1	1.92	0.53
4:O:72:PRO:HB2	6:Q:139:ALA:HB2	1.90	0.53
2:B:65:LEU:O	2:B:69:ARG:HG2	2.09	0.53
10:U:18:LEU:O	10:U:82:LYS:HA	2.08	0.52
1:A:373:GLN:HG3	1:A:374:LEU:N	2.24	0.52
2:B:49:HIS:HE1	2:B:130:ASP:OD1	1.93	0.52
2:B:83:ASP:HB2	2:B:86:TYR:H	1.74	0.52
1:A:86:ALA:HB2	1:A:119:PHE:CZ	2.44	0.52
3:N:301:VAL:O	3:N:304:VAL:HG12	2.09	0.52
10:U:38:ILE:HD13	10:U:112:TRP:HH2	1.73	0.52
5:E:134:MET:HG3	10:J:31:SER:CB	2.35	0.52
6:F:91:GLY:O	6:F:95:VAL:HG13	2.10	0.52
3:N:4:ARG:HE	3:N:14:ASN:ND2	2.07	0.52
5:P:115:PRO:HD2	5:P:158:ILE:HD11	1.91	0.52
2:M:260:LEU:O	2:M:271:ILE:HD11	2.10	0.52
1:L:252:ARG:HD3	1:L:254:ASP:OD1	2.10	0.52
1:L:241:LYS:HD2	1:L:241:LYS:N	2.24	0.52
2:B:35:VAL:CG1	2:B:179:VAL:HG12	2.40	0.52
1:A:181:THR:O	1:A:185:LEU:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:69:LEU:HD23	6:F:128:PHE:CD1	2.45	0.52
15:C:4002:HEM:HBB2	15:C:4002:HEM:HMB1	1.92	0.52
1:A:179:ARG:HG2	1:A:179:ARG:HH21	1.74	0.52
3:C:184:TYR:CD1	15:C:4001:HEM:HBC1	2.45	0.51
3:N:4:ARG:HE	3:N:14:ASN:HD21	1.56	0.51
3:N:335:LEU:O	3:N:339:ILE:HG12	2.10	0.51
3:C:25:SER:OG	7:G:79:HIS:HD2	1.93	0.51
1:L:182:LEU:O	1:L:186:GLU:HG2	2.10	0.51
4:O:231:ASP:OD1	4:O:244:THR:HG23	2.09	0.51
10:U:49:VAL:CG1	10:U:68:LEU:HD23	2.41	0.51
20:O:4114:7PH:H25	20:O:4114:7PH:H29	1.93	0.51
1:A:306:ILE:HA	1:A:311:LEU:HD22	1.92	0.51
4:O:92:ARG:HG2	4:O:236:TYR:CD2	2.46	0.51
11:V:29:ILE:HG22	11:V:92:ILE:HD12	1.93	0.51
10:U:59:ASN:HD22	10:U:59:ASN:C	2.13	0.51
12:W:36:LYS:HB3	23:W:7422:HOH:O	2.10	0.51
18:C:4031:CN6:HC	23:C:6590:HOH:O	2.11	0.51
2:B:264:LEU:HD12	2:B:317:ALA:HB2	1.92	0.51
2:B:115:LYS:HB2	2:B:118:GLU:HG3	1.92	0.51
2:B:232:ARG:NH1	2:M:164:VAL:HG21	2.26	0.51
2:M:62:ARG:HH21	2:M:62:ARG:CG	2.17	0.51
2:M:315:SER:HB3	2:M:344:LYS:HA	1.93	0.51
3:C:58:ILE:H	3:C:173:ASN:HD22	1.58	0.51
12:W:28:THR:HG23	12:W:36:LYS:HE2	1.93	0.51
2:M:247:LYS:O	2:M:250:LEU:HD22	2.10	0.51
10:J:107:TYR:H	11:K:91:HIS:CD2	2.29	0.51
2:M:298:SER:O	2:M:302:LYS:HB2	2.11	0.51
11:K:17:ASP:HB2	11:K:18:ARG:HH21	1.75	0.51
2:B:183:GLU:HB2	2:B:213:LYS:O	2.10	0.51
2:B:62:ARG:HH21	2:B:62:ARG:CG	2.24	0.50
4:D:92:ARG:HG2	4:D:236:TYR:CD2	2.45	0.50
4:O:135:ASP:OD2	4:O:146:LYS:HE2	2.11	0.50
2:B:364:TYR:CZ	2:M:152:ARG:HG2	2.46	0.50
2:B:255:VAL:HG12	2:B:321:THR:HG21	1.94	0.50
2:M:26:THR:HG21	2:M:191:ASN:HD21	1.77	0.50
1:A:350:GLN:O	1:A:353:ARG:HB2	2.12	0.50
10:U:38:ILE:HD13	10:U:112:TRP:CH2	2.46	0.50
11:V:21:ILE:HG22	11:V:22:SER:H	1.75	0.50
1:A:67:ASN:HD22	1:A:181:THR:HG23	1.76	0.50
10:U:87:THR:O	10:U:120:VAL:HG21	2.10	0.50
2:B:246:ASN:HB2	2:B:249:SER:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:61:ILE:HB	8:H:62:PRO:HD3	1.92	0.50
3:N:320:VAL:HG13	8:S:58:TYR:HE2	1.76	0.50
2:M:308:LEU:CB	2:M:348:LEU:HD22	2.41	0.50
1:L:179:ARG:HD2	1:L:179:ARG:H	1.76	0.50
5:P:44:LYS:HB3	8:S:35:LYS:HG3	1.92	0.50
1:A:239:LYS:HD2	1:A:239:LYS:N	2.25	0.50
1:A:345:HIS:O	1:A:349:LYS:HB2	2.12	0.50
1:L:63:ASN:N	1:L:66:ASN:ND2	2.44	0.50
11:K:37:GLN:HB2	11:K:47:LEU:HD11	1.91	0.50
3:C:107:ARG:NH2	3:C:107:ARG:HG3	2.27	0.50
1:A:99:ARG:HD3	1:A:174:LEU:CD1	2.41	0.50
1:A:214:ILE:HD12	1:A:214:ILE:O	2.11	0.50
7:R:97:GLN:NE2	7:R:97:GLN:H	2.10	0.50
1:A:164:LEU:HD13	1:A:327:LEU:HD13	1.94	0.50
4:O:286:TRP:CD2	5:P:59:MET:HG3	2.46	0.50
1:A:198:ASN:O	1:A:202:LEU:HD21	2.11	0.50
5:P:38:ASN:HD21	5:P:40:ASP:CG	2.15	0.50
1:A:172:THR:HG21	1:A:243:ALA:H	1.77	0.50
3:C:313:VAL:HG22	3:C:319:LYS:HE3	1.94	0.50
8:H:35:LYS:O	8:H:37:LEU:N	2.34	0.50
3:C:313:VAL:HG22	3:C:319:LYS:CE	2.43	0.49
3:C:229:ASP:O	3:C:233:VAL:HG23	2.12	0.49
1:L:238:LEU:N	1:L:238:LEU:HD22	2.27	0.49
1:A:350:GLN:HE22	1:A:353:ARG:HH21	1.59	0.49
4:O:301:VAL:CG2	8:S:25:THR:HB	2.42	0.49
1:L:375:GLY:HA3	2:M:28:ILE:HG13	1.93	0.49
1:A:397:LYS:HG3	1:A:399:SER:O	2.13	0.49
4:O:163:GLN:NE2	4:O:163:GLN:H	2.11	0.49
3:C:222:HIS:O	3:C:223:SER:HB2	2.13	0.49
3:C:14:ASN:HD22	3:C:18:ILE:HB	1.76	0.49
3:C:326:PHE:CZ	17:C:4010:8PE:H34A	2.47	0.49
1:L:29:VAL:HG12	1:L:30:THR:H	1.75	0.49
3:C:110:ARG:NH2	3:C:205:GLY:O	2.46	0.49
3:C:77:ILE:O	3:C:81:LEU:HB2	2.13	0.49
1:L:57:SER:HA	1:L:61:ASN:ND2	2.28	0.49
1:A:265:VAL:HG21	1:A:426:LEU:HD13	1.94	0.49
11:K:103:LYS:HG2	11:K:104:LEU:H	1.78	0.49
1:A:275:TYR:CZ	1:A:279:LYS:HE2	2.46	0.49
2:M:310:LYS:HE3	2:M:312:LYS:HB3	1.94	0.49
3:C:104:GLY:HA2	3:C:106:TYR:CE2	2.48	0.49
11:V:11:LEU:HG	11:V:12:ALA:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:326:PHE:HZ	17:C:4010:8PE:H34A	1.78	0.49
10:U:7:SER:OG	10:U:21:THR:HG23	2.12	0.49
1:A:235:LYS:HB2	1:A:235:LYS:NZ	2.26	0.49
11:K:12:ALA:HA	11:K:105:GLU:O	2.13	0.49
3:N:76:TYR:CG	4:O:262:GLU:HG3	2.48	0.49
1:L:306:ILE:HA	1:L:311:LEU:HD22	1.94	0.49
2:M:62:ARG:NH2	2:M:67:LEU:HD13	2.28	0.49
1:L:172:THR:HG23	1:L:173:PRO:HD2	1.95	0.49
12:W:26:CYS:HB3	12:W:37:VAL:HB	1.94	0.49
1:A:302:LEU:HB2	1:A:350:GLN:HG3	1.95	0.49
3:N:320:VAL:HG23	23:N:6971:HOH:O	2.13	0.49
5:P:168:GLY:HA2	5:P:176:TRP:CD1	2.47	0.49
7:G:91:ASN:H	7:G:91:ASN:ND2	2.10	0.49
1:A:122:GLN:HG3	1:A:126:GLN:NE2	2.28	0.48
2:M:44:LYS:O	2:M:47:VAL:HG23	2.13	0.48
18:C:4031:CN6:O14	4:D:288:LYS:NZ	2.46	0.48
5:E:93:LYS:HE3	5:E:213:ILE:HD11	1.94	0.48
1:A:247:SER:O	1:A:432:ALA:HA	2.13	0.48
12:W:20:LYS:HA	12:W:24:GLN:HG2	1.94	0.48
10:J:87:THR:HG22	10:J:88:THR:N	2.28	0.48
1:A:280:LEU:HD13	1:A:413:ILE:HG21	1.96	0.48
1:L:230:LEU:HD13	1:L:231:GLN:HG3	1.94	0.48
2:M:347:LYS:O	2:M:348:LEU:HB2	2.12	0.48
5:E:122:THR:O	5:E:126:ILE:HG13	2.13	0.48
1:A:156:HIS:HD2	1:A:159:ARG:HH21	1.61	0.48
1:A:30:THR:HB	1:A:216:HIS:CD2	2.48	0.48
2:B:193:VAL:O	2:B:193:VAL:HG23	2.12	0.48
1:A:172:THR:CG2	1:A:242:ALA:HA	2.43	0.48
1:L:429:GLN:HA	1:L:429:GLN:OE1	2.14	0.48
1:L:73:TRP:CE3	1:L:76:ILE:HD11	2.47	0.48
2:B:52:ASN:ND2	2:B:80:SER:OG	2.45	0.48
1:L:172:THR:HG21	1:L:243:ALA:H	1.78	0.48
1:A:86:ALA:HB2	1:A:119:PHE:CE1	2.48	0.48
3:C:220:PRO:HB2	23:C:7439:HOH:O	2.13	0.48
3:C:234:PHE:CZ	4:D:280:LEU:HG	2.49	0.48
1:A:58:GLY:H	1:A:61:ASN:ND2	2.02	0.48
4:O:136:ASP:HB3	4:O:145:LYS:HG3	1.96	0.48
7:R:53:ASN:ND2	7:R:56:MET:H	2.11	0.48
5:E:146:ARG:CZ	5:E:202:ILE:HD11	2.44	0.48
1:A:36:ILE:HA	1:A:203:ASN:HD21	1.79	0.48
2:B:35:VAL:HG12	2:B:179:VAL:HG12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:ASN:O	1:A:125:ILE:HB	2.14	0.48
11:V:50:TYR:O	11:V:51:THR:HG22	2.13	0.48
2:B:104:ALA:O	2:B:108:VAL:HG23	2.14	0.48
2:M:305:VAL:O	2:M:309:LYS:HG2	2.14	0.48
1:L:141:LYS:HE3	1:L:186:GLU:HA	1.94	0.48
6:Q:91:GLY:O	6:Q:95:VAL:HG13	2.14	0.48
4:D:286:TRP:HZ3	5:E:56:ALA:HA	1.79	0.47
17:N:4110:8PE:H3AA	17:N:4110:8PE:H37A	1.66	0.47
2:B:315:SER:N	2:B:316:PRO:HD3	2.29	0.47
4:O:109:ARG:HG3	4:O:178:SER:HB2	1.96	0.47
5:E:65:LEU:HD21	9:I:24:GLY:C	2.35	0.47
6:Q:90:GLU:HG2	6:Q:133:TYR:CE1	2.50	0.47
10:J:49:VAL:CG1	10:J:68:LEU:HD23	2.44	0.47
11:K:2:ILE:HD12	11:K:2:ILE:N	2.30	0.47
5:E:187:ILE:HG13	5:E:187:ILE:O	2.14	0.47
2:M:318:ILE:O	2:M:321:THR:HG22	2.14	0.47
3:N:222:HIS:O	3:N:223:SER:HB2	2.14	0.47
1:L:76:ILE:HG23	1:L:140:THR:HG21	1.95	0.47
1:L:28:GLU:O	1:L:41:GLU:HG3	2.13	0.47
5:P:43:LEU:HD21	8:S:29:VAL:HG11	1.96	0.47
10:J:18:LEU:O	10:J:82:LYS:HA	2.14	0.47
4:D:203:PRO:HG2	4:D:206:VAL:HG21	1.96	0.47
1:L:67:ASN:ND2	1:L:180:GLY:HA2	2.29	0.47
4:D:227:ARG:HH11	4:D:244:THR:HG21	1.80	0.47
5:E:154:ILE:HD12	5:E:205:TYR:CE2	2.50	0.47
1:A:141:LYS:O	1:A:145:LEU:HB2	2.15	0.47
1:L:66:ASN:HD22	1:L:66:ASN:H	1.63	0.47
11:V:75:ILE:CG2	11:V:76:SER:H	2.18	0.47
1:L:169:PHE:HB3	1:L:172:THR:HG22	1.96	0.47
14:A:4021:UMQ:HC1	9:I:18:VAL:CG1	2.45	0.47
1:L:67:ASN:HD21	1:L:177:PRO:HG2	1.80	0.47
5:E:51:LYS:HD2	8:H:36:PRO:HG3	1.96	0.47
15:N:4022:HEM:HBC2	15:N:4022:HEM:HMC2	1.95	0.47
3:C:208:ASN:HD22	3:C:210:LEU:N	2.09	0.47
1:L:72:LEU:HD22	1:L:188:LEU:HD23	1.97	0.47
11:K:2:ILE:HG22	11:K:3:GLU:N	2.29	0.47
2:B:317:ALA:O	2:B:321:THR:HG22	2.15	0.47
4:O:225:MET:HB2	15:O:4023:HEM:C1D	2.49	0.47
7:G:45:PHE:O	7:G:48:LEU:HB2	2.15	0.47
2:M:233:PHE:HB3	2:M:357:GLY:HA2	1.97	0.47
4:D:92:ARG:O	4:D:96:VAL:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:69:LEU:HD12	4:D:217:TYR:CE2	2.49	0.47
3:N:17:ILE:HG23	3:N:226:ILE:HD11	1.97	0.47
3:C:332:ASN:HD21	3:C:355:ALA:HA	1.79	0.47
2:B:43:THR:HG22	2:B:178:LYS:HZ2	1.80	0.47
2:M:152:ARG:O	2:M:153:LYS:HB2	2.14	0.47
2:B:271:ILE:HG22	2:B:289:VAL:HG22	1.97	0.47
3:C:323:LYS:NZ	8:H:55:GLN:HE22	2.13	0.47
10:U:99:SER:HB3	10:U:109:MET:HG2	1.97	0.46
10:U:21:THR:HB	10:U:80:PHE:HD2	1.79	0.46
1:A:156:HIS:HD2	1:A:159:ARG:NH2	2.13	0.46
5:P:106:ASN:ND2	5:P:119:ARG:HH21	2.14	0.46
10:J:20:LEU:HD12	10:J:81:LEU:HD23	1.97	0.46
1:A:261:ILE:HG13	1:A:262:SER:N	2.29	0.46
2:M:347:LYS:H	2:M:347:LYS:CD	2.07	0.46
3:C:208:ASN:HB2	3:C:209:PRO:HD2	1.96	0.46
2:B:43:THR:HG22	2:B:178:LYS:NZ	2.31	0.46
10:U:37:TRP:CE2	10:U:81:LEU:HB2	2.50	0.46
5:E:114:LYS:HD3	5:E:114:LYS:H	1.81	0.46
1:L:252:ARG:HD2	8:S:21:GLN:HB2	1.96	0.46
5:E:146:ARG:NH2	5:E:202:ILE:HD11	2.31	0.46
1:A:291:PHE:HZ	1:A:335:ARG:HH11	1.63	0.46
3:C:35:LEU:HD13	23:C:5040:HOH:O	2.15	0.46
8:H:3:PRO:HG3	8:S:12:TRP:CZ2	2.49	0.46
4:D:286:TRP:CZ3	5:E:56:ALA:HA	2.51	0.46
1:L:109:LEU:HB3	1:L:110:PRO:HD2	1.97	0.46
1:A:37:VAL:HG13	1:A:207:VAL:HA	1.97	0.46
16:C:4005:SMA:H39	16:C:4005:SMA:H33	1.97	0.46
7:G:43:LEU:HD21	7:G:78:ALA:HB1	1.97	0.46
11:K:4:LEU:HD23	11:K:88:CYS:SG	2.55	0.46
2:B:251:ALA:HB2	2:B:339:ASN:HB3	1.97	0.46
4:D:109:ARG:HG3	4:D:178:SER:HB2	1.98	0.46
2:B:315:SER:HB2	2:B:318:ILE:HD13	1.96	0.46
6:Q:87:ASN:O	6:Q:92:LYS:HE2	2.15	0.46
1:A:270:VAL:HG21	1:A:396:ILE:HD13	1.98	0.46
1:A:102:GLN:HE22	1:A:196:PHE:HE1	1.63	0.46
11:K:37:GLN:O	11:K:44:ILE:HA	2.16	0.46
4:O:286:TRP:CZ3	5:P:56:ALA:HA	2.50	0.46
3:C:193:MET:HE2	3:C:196:MET:SD	2.56	0.46
2:B:146:LEU:O	2:B:150:THR:HG23	2.16	0.46
4:D:223:ILE:HG12	4:D:225:MET:H	1.79	0.46
5:E:55:TYR:O	5:E:59:MET:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:277:LEU:HD21	20:D:4014:7PH:H33A	1.99	0.45
5:E:213:ILE:HG12	5:E:213:ILE:O	2.16	0.45
5:P:51:LYS:HE2	5:P:55:TYR:HE1	1.81	0.45
3:C:263:LEU:HD22	5:P:115:PRO:HB3	1.98	0.45
10:U:36:ASN:OD1	10:U:51:TYR:HB3	2.16	0.45
2:M:30:THR:HG21	2:M:90:LYS:HE2	1.98	0.45
4:O:268:ARG:NH1	9:T:33:ASP:OD1	2.49	0.45
6:F:117:LEU:C	6:F:119:HIS:H	2.19	0.45
2:B:53:ARG:HB3	2:B:123:VAL:HG13	1.98	0.45
1:L:130:ASN:N	1:L:130:ASN:ND2	2.64	0.45
1:L:230:LEU:O	1:L:231:GLN:HB2	2.16	0.45
1:A:57:SER:HA	1:A:61:ASN:ND2	2.30	0.45
10:J:99:SER:HA	10:J:109:MET:HA	1.97	0.45
1:L:130:ASN:HD22	1:L:130:ASN:H	1.63	0.45
2:B:152:ARG:HD3	2:B:224:PHE:CD1	2.52	0.45
2:M:313:ASP:C	2:M:315:SER:H	2.20	0.45
5:P:146:ARG:CZ	5:P:202:ILE:HD11	2.46	0.45
1:L:181:THR:O	1:L:185:LEU:HB2	2.17	0.45
7:G:53:ASN:ND2	7:G:56:MET:H	2.13	0.45
10:U:87:THR:HG22	10:U:88:THR:N	2.30	0.45
2:B:313:ASP:HB3	2:B:344:LYS:O	2.16	0.45
2:B:141:SER:O	2:B:145:GLN:HG2	2.16	0.45
4:D:113:ARG:HG2	4:D:151:LEU:O	2.17	0.45
11:K:93:LYS:HB3	11:K:93:LYS:NZ	2.31	0.45
7:G:41:LEU:HB2	7:G:43:LEU:HD23	1.99	0.45
14:A:4021:UMQ:HC1	9:I:18:VAL:HG12	1.97	0.45
1:L:88:LYS:HG3	2:M:264:LEU:HD21	1.99	0.45
11:V:93:LYS:HZ3	11:V:94:PHE:N	2.08	0.45
5:E:100:ALA:O	5:E:102:PRO:HD3	2.17	0.45
11:K:13:ALA:O	11:K:106:ILE:HG22	2.16	0.45
6:F:94:LEU:HB3	6:F:130:LEU:HD23	1.98	0.45
3:N:313:VAL:HG22	3:N:319:LYS:HE3	1.99	0.45
2:M:251:ALA:HB2	2:M:339:ASN:HB3	1.99	0.45
4:O:134:TYR:OH	4:O:156:PRO:HD3	2.17	0.45
1:A:74:LYS:HG3	1:A:95:SER:HB3	1.98	0.45
2:M:289:VAL:HG12	2:M:297:VAL:HG13	1.99	0.45
7:G:26:VAL:HG12	7:G:30:ASN:ND2	2.31	0.45
1:A:239:LYS:HB2	1:A:240:LYS:H	1.54	0.45
10:U:21:THR:HB	10:U:80:PHE:CD2	2.52	0.45
2:M:251:ALA:O	2:M:255:VAL:HG13	2.16	0.45
10:J:91:THR:HG23	10:J:119:THR:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:ASN:HA	1:A:383:PRO:HD3	1.78	0.45
4:D:147:ARG:NH2	4:D:150:LYS:HE3	2.32	0.45
5:E:120:HIS:ND1	5:E:152:TRP:CH2	2.85	0.45
10:J:37:TRP:CE2	10:J:81:LEU:HB2	2.53	0.45
7:R:5:PHE:CD1	7:R:107:ILE:HG21	2.52	0.45
11:V:32:PHE:CD2	11:V:32:PHE:N	2.84	0.45
2:M:205:LEU:H	2:M:205:LEU:HD12	1.82	0.45
1:A:66:ASN:HD22	1:A:66:ASN:N	2.06	0.44
2:M:246:ASN:ND2	2:M:246:ASN:N	2.63	0.44
10:U:82:LYS:HE2	10:U:84:ASN:OD1	2.16	0.44
2:M:262:SER:HB3	2:M:320:TYR:CE1	2.52	0.44
11:K:29:ILE:HA	11:K:92:ILE:HG21	1.99	0.44
12:W:57:TYR:CD1	12:W:61:ASN:ND2	2.85	0.44
1:L:97:ILE:HD13	1:L:102:GLN:HG3	1.98	0.44
1:A:73:TRP:CZ3	1:A:76:ILE:HD11	2.53	0.44
1:A:234:THR:HG22	1:A:235:LYS:N	2.32	0.44
6:F:104:ARG:HG2	6:F:108:GLN:HE21	1.82	0.44
11:K:39:LYS:NZ	11:K:81:GLU:HG2	2.32	0.44
1:A:76:ILE:CG2	1:A:140:THR:HG21	2.47	0.44
3:C:104:GLY:O	3:C:107:ARG:HG2	2.18	0.44
4:D:227:ARG:NH1	4:D:244:THR:HG21	2.33	0.44
7:G:97:GLN:NE2	7:G:97:GLN:H	2.15	0.44
2:B:215:LEU:HB2	23:B:7003:HOH:O	2.16	0.44
1:L:302:LEU:HB2	1:L:350:GLN:HG3	2.00	0.44
1:A:62:GLU:OE1	1:A:67:ASN:HA	2.18	0.44
10:U:34:TYR:HB2	10:U:99:SER:OG	2.18	0.44
2:B:145:GLN:OE1	2:B:229:ASN:ND2	2.49	0.44
2:M:205:LEU:N	2:M:205:LEU:HD12	2.33	0.44
10:J:12:VAL:O	10:J:120:VAL:HA	2.18	0.44
5:E:134:MET:HG2	23:J:7001:HOH:O	2.16	0.44
7:G:18:SER:OG	7:G:21:LEU:HD23	2.18	0.44
4:O:111:ALA:HA	4:O:154:TYR:HA	2.00	0.44
1:A:127:GLN:HA	1:A:130:ASN:HD22	1.82	0.44
1:A:88:LYS:HE3	2:B:264:LEU:HD22	2.00	0.44
1:A:141:LYS:HE3	1:A:186:GLU:HA	2.00	0.44
7:G:120:LEU:O	7:G:123:ILE:HG12	2.18	0.44
1:A:109:LEU:HB3	1:A:110:PRO:HD2	2.00	0.44
1:A:160:VAL:HG21	1:A:436:THR:HG22	1.99	0.43
2:B:232:ARG:NH1	2:M:164:VAL:CG2	2.81	0.43
1:L:429:GLN:HE22	9:T:13:ARG:NH2	2.16	0.43
2:B:326:ALA:C	2:B:328:GLN:H	2.20	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:V:32:PHE:N	11:V:32:PHE:HD2	2.15	0.43
3:C:157:VAL:O	3:C:161:ILE:HG12	2.18	0.43
4:O:76:TRP:CZ2	4:O:188:CYS:HB3	2.53	0.43
1:A:248:GLU:HA	1:A:433:ILE:O	2.19	0.43
2:M:220:GLU:HA	2:M:221:PRO:HD3	1.83	0.43
10:J:51:TYR:C	10:J:51:TYR:CD2	2.91	0.43
5:P:107:VAL:CG1	5:P:118:ILE:HB	2.48	0.43
3:C:193:MET:HE2	3:C:193:MET:HA	1.99	0.43
3:C:80:TYR:CE1	3:C:248:PRO:HB2	2.53	0.43
2:M:56:PHE:CZ	2:M:78:PHE:HB3	2.53	0.43
3:N:125:ILE:HG22	16:N:4025:SMA:H37	2.00	0.43
2:B:250:LEU:HD21	2:B:336:ILE:HD13	2.00	0.43
10:U:65:LYS:HA	10:U:68:LEU:HD11	2.00	0.43
8:S:3:PRO:HA	8:S:4:PRO:HD3	1.86	0.43
1:L:311:LEU:HB3	1:L:343:LEU:HG	2.00	0.43
2:B:220:GLU:HA	2:B:221:PRO:HD3	1.84	0.43
10:U:49:VAL:HG12	10:U:68:LEU:HD23	2.01	0.43
5:E:132:VAL:HG21	5:E:192:ARG:NH1	2.34	0.43
5:P:93:LYS:HG2	5:P:213:ILE:HD11	2.00	0.43
10:U:61:ASN:ND2	10:U:63:SER:H	2.12	0.43
3:N:253:HIS:HE1	3:N:268:SER:O	2.01	0.43
11:K:8:PRO:O	11:K:102:THR:HG23	2.19	0.43
3:C:315:GLY:HA3	23:C:6558:HOH:O	2.17	0.43
7:R:63:LEU:HD12	7:R:64:PRO:HD2	2.00	0.43
8:H:48:SER:C	8:H:50:ARG:H	2.21	0.43
2:M:204:SER:OG	2:M:206:LEU:HB2	2.18	0.43
18:C:4031:CN6:H57	18:C:4031:CN6:H3A	1.65	0.43
10:U:51:TYR:CD2	10:U:51:TYR:C	2.91	0.43
1:A:430:ASP:OD2	1:A:449:ARG:NH2	2.51	0.43
1:A:366:ALA:O	1:A:370:LEU:HB2	2.18	0.43
1:L:169:PHE:O	1:L:172:THR:HB	2.18	0.43
5:P:181:HIS:HB2	21:P:4024:FES:S1	2.58	0.43
1:A:43:ASN:HA	1:A:44:PRO:HD2	1.85	0.43
10:J:41:PHE:HB3	10:J:42:PRO:HD2	2.00	0.43
4:D:187:GLY:O	4:D:191:ILE:HG12	2.19	0.43
11:K:103:LYS:HG2	11:K:104:LEU:N	2.34	0.43
7:G:39:LYS:HG2	7:G:94:ILE:HB	2.00	0.43
2:M:49:HIS:HE1	2:M:130:ASP:OD1	2.02	0.42
1:L:74:LYS:HG3	1:L:95:SER:CB	2.49	0.42
2:B:121:GLU:OE2	7:R:62:ARG:HD2	2.19	0.42
4:O:86:ASP:HA	9:T:47:LYS:HG2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:42:ALA:HB1	2:B:47:VAL:HG12	2.01	0.42
3:C:216:LEU:HD12	3:C:216:LEU:N	2.33	0.42
2:B:30:THR:CG2	2:B:190:GLU:HB3	2.46	0.42
1:L:207:VAL:HG21	1:L:394:VAL:HG23	2.00	0.42
11:K:7:THR:HG23	11:K:22:SER:OG	2.19	0.42
10:J:98:ARG:O	10:J:109:MET:HA	2.19	0.42
11:K:17:ASP:HB2	11:K:18:ARG:NH2	2.34	0.42
10:U:12:VAL:O	10:U:120:VAL:HA	2.19	0.42
2:M:251:ALA:CB	2:M:339:ASN:HB3	2.49	0.42
5:P:93:LYS:HG3	5:P:214:VAL:O	2.18	0.42
1:L:401:LEU:HB3	23:L:7297:HOH:O	2.18	0.42
3:N:138:GLN:HA	3:N:138:GLN:OE1	2.20	0.42
1:A:76:ILE:HG23	1:A:140:THR:HG21	2.01	0.42
2:M:254:GLU:CG	2:M:278:LYS:HE3	2.50	0.42
1:L:42:HIS:HB2	23:L:7033:HOH:O	2.18	0.42
2:B:270:LEU:HB3	2:B:304:ILE:HD11	2.01	0.42
2:B:52:ASN:HD21	2:B:80:SER:C	2.23	0.42
2:B:117:HIS:HB3	7:R:62:ARG:HG2	2.02	0.42
11:K:79:GLU:HA	11:K:80:PRO:HA	1.74	0.42
2:M:347:LYS:CG	2:M:348:LEU:H	2.23	0.42
10:J:61:ASN:HD22	10:J:61:ASN:C	2.23	0.42
10:J:38:ILE:HA	10:J:49:VAL:HG23	2.01	0.42
7:G:62:ARG:HG2	2:M:117:HIS:HB3	2.01	0.42
4:D:111:ALA:HA	4:D:154:TYR:HA	2.01	0.42
1:L:386:ASP:O	1:L:390:LEU:HB2	2.20	0.42
1:L:58:GLY:H	1:L:61:ASN:ND2	2.10	0.42
1:L:169:PHE:CD1	1:L:174:LEU:HB3	2.55	0.42
4:D:147:ARG:HG2	4:D:148:PRO:O	2.20	0.42
11:K:4:LEU:CD2	11:K:88:CYS:SG	3.08	0.42
8:H:61:ILE:O	8:H:65:ILE:HG13	2.20	0.42
12:W:18:LEU:HD23	12:W:103:LEU:HB2	2.02	0.42
3:N:216:LEU:HD12	3:N:216:LEU:N	2.35	0.42
1:L:447:ARG:NH1	3:N:18:ILE:HG22	2.34	0.42
6:Q:81:LEU:HB3	6:Q:138:THR:HG22	2.02	0.42
1:A:386:ASP:O	1:A:390:LEU:HB2	2.19	0.42
4:O:123:GLU:CD	4:O:123:GLU:H	2.23	0.42
5:P:120:HIS:ND1	5:P:152:TRP:CH2	2.87	0.42
1:A:344:ILE:HG21	1:A:448:ILE:HD12	2.02	0.42
7:R:115:LYS:HE3	7:R:119:GLU:OE2	2.20	0.42
2:B:332:VAL:HG12	2:B:332:VAL:O	2.20	0.42
10:U:6:GLU:HG2	10:U:96:CYS:SG	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:GLU:CD	2:B:53:ARG:HH12	2.23	0.41
2:B:39:SER:OG	2:B:84:ARG:HA	2.20	0.41
2:M:338:LEU:HD22	2:M:338:LEU:H	1.84	0.41
12:W:70:GLU:H	12:W:70:GLU:CD	2.22	0.41
3:N:77:ILE:O	3:N:81:LEU:HB2	2.19	0.41
18:C:4031:CN6:HAA	7:G:85:HIS:CE1	2.55	0.41
18:N:4131:CN6:H57	18:N:4131:CN6:H3A	1.81	0.41
2:M:44:LYS:HB2	2:M:47:VAL:CG2	2.50	0.41
5:E:125:GLU:HB3	5:E:187:ILE:HG12	2.02	0.41
10:U:36:ASN:HD21	10:U:99:SER:CB	2.33	0.41
11:K:19:VAL:HG12	11:K:75:ILE:HB	2.02	0.41
4:D:256:ASN:C	4:D:256:ASN:HD22	2.23	0.41
4:D:76:TRP:CZ2	4:D:188:CYS:HB3	2.55	0.41
2:B:66:LYS:HE3	2:B:70:GLU:OE2	2.20	0.41
2:B:53:ARG:HD3	2:B:130:ASP:OD1	2.19	0.41
5:E:165:VAL:HG23	3:N:142:TRP:CH2	2.55	0.41
11:K:46:LEU:HD23	11:K:55:HIS:CD2	2.54	0.41
3:C:99:LYS:HD2	3:C:99:LYS:C	2.40	0.41
3:C:313:VAL:CG2	3:C:319:LYS:HE3	2.50	0.41
2:B:98:LEU:O	2:B:102:VAL:HG23	2.20	0.41
1:A:447:ARG:NH1	3:C:18:ILE:HG22	2.36	0.41
14:L:4121:UMQ:HC1	9:T:18:VAL:HG13	2.02	0.41
1:L:102:GLN:HE21	1:L:102:GLN:HB2	1.68	0.41
7:G:91:ASN:H	7:G:91:ASN:HD22	1.69	0.41
11:K:48:ILE:HD13	11:K:54:LEU:HA	2.02	0.41
7:R:46:ASP:HB2	7:R:102:TYR:CE2	2.55	0.41
11:V:4:LEU:HD23	11:V:88:CYS:SG	2.61	0.41
2:B:183:GLU:HG2	2:B:211:ALA:HB1	2.03	0.41
1:L:379:GLU:OE1	2:M:26:THR:HB	2.21	0.41
7:G:127:LYS:HD3	7:G:127:LYS:N	2.36	0.41
10:J:29:ILE:H	10:J:77:ASN:HD21	1.69	0.41
11:K:58:VAL:HA	11:K:59:PRO:HD3	1.86	0.41
1:A:220:VAL:O	1:A:224:GLU:HB2	2.21	0.41
5:E:38:ASN:HD21	5:E:40:ASP:CG	2.24	0.41
2:M:230:ARG:HG2	2:M:230:ARG:HH21	1.86	0.41
3:N:107:ARG:NH1	3:N:311:SER:O	2.54	0.41
3:N:58:ILE:HD11	3:N:136:TYR:CZ	2.55	0.41
12:W:58:THR:HB	15:W:4026:HEM:O2D	2.20	0.41
1:A:252:ARG:HG3	1:A:439:ILE:HG13	2.02	0.41
3:C:193:MET:CE	3:C:196:MET:SD	3.09	0.41
1:A:364:GLU:HG3	7:R:125:VAL:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:256:ASN:HD22	4:O:256:ASN:C	2.24	0.41
3:C:178:ARG:HE	3:C:178:ARG:HB3	1.72	0.41
2:B:46:GLY:HA3	2:B:161:TYR:HA	2.03	0.41
18:C:4031:CN6:H2'	18:C:4031:CN6:H52A	1.68	0.41
4:D:92:ARG:HG2	4:D:236:TYR:CE2	2.56	0.41
1:L:72:LEU:HD13	1:L:144:VAL:HG21	2.03	0.41
2:B:31:LEU:HD21	2:B:197:LEU:HD11	2.03	0.41
1:A:179:ARG:NH2	1:A:179:ARG:HG2	2.35	0.41
10:J:87:THR:HG22	10:J:89:GLU:H	1.85	0.41
2:B:41:TYR:HD2	2:B:215:LEU:HD13	1.86	0.41
1:L:43:ASN:HA	1:L:44:PRO:HD2	1.89	0.41
2:M:193:VAL:HG23	2:M:196:ASP:HB2	2.02	0.41
1:A:266:GLU:O	1:A:425:ARG:HG3	2.21	0.41
2:M:39:SER:OG	2:M:84:ARG:HA	2.20	0.41
11:V:34:ASN:ND2	11:V:49:TYR:HA	2.36	0.41
3:C:234:PHE:CE2	4:D:280:LEU:HG	2.55	0.41
1:A:74:LYS:HE3	1:A:95:SER:O	2.21	0.41
8:H:48:SER:O	8:H:49:PHE:HB2	2.21	0.41
12:W:43:GLY:N	12:W:111:ALA:O	2.53	0.41
1:L:318:PHE:HB2	1:L:320:LEU:HD13	2.03	0.41
3:N:314:ARG:HD3	23:N:5535:HOH:O	2.20	0.41
1:L:74:LYS:HB2	1:L:97:ILE:HD11	2.04	0.40
2:B:336:ILE:HD12	2:B:336:ILE:N	2.30	0.40
12:W:37:VAL:O	15:W:4026:HEM:HMD3	2.22	0.40
5:E:114:LYS:N	5:E:114:LYS:HD3	2.36	0.40
8:H:3:PRO:HG3	8:S:12:TRP:CE2	2.56	0.40
5:E:164:CYS:HB2	5:E:178:CYS:SG	2.62	0.40
4:O:212:SER:O	13:O:4146:SUC:H4'	2.22	0.40
1:L:46:ALA:HB3	1:L:213:ASN:HB3	2.03	0.40
4:O:273:THR:OG1	20:O:4114:7PH:H2	2.22	0.40
2:B:146:LEU:HA	2:B:146:LEU:HD13	1.93	0.40
7:R:43:LEU:HD21	7:R:78:ALA:CB	2.51	0.40
10:U:29:ILE:N	10:U:77:ASN:HD21	2.06	0.40
2:B:364:TYR:CE1	2:M:152:ARG:HG2	2.56	0.40
11:K:4:LEU:HD21	11:K:33:LEU:HD11	2.04	0.40
12:W:96:LYS:HD3	12:W:98:LYS:HZ3	1.85	0.40
10:J:10:GLY:HA2	10:J:118:VAL:HG12	2.02	0.40
8:S:88:GLU:O	8:S:92:VAL:HG22	2.20	0.40
2:B:30:THR:OG1	2:B:90:LYS:HE3	2.22	0.40
10:U:54:ASN:H	10:U:54:ASN:ND2	2.18	0.40
1:A:271:ASN:HD21	1:A:397:LYS:NZ	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:145:GLN:HB3	2:B:354:VAL:HG11	2.03	0.40
3:C:20:SER:HA	3:C:21:PRO:HD3	1.91	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	429/431 (100%)	395 (92%)	33 (8%)	1 (0%)	52 75
1	L	429/431 (100%)	393 (92%)	32 (8%)	4 (1%)	21 37
2	B	350/352 (99%)	310 (89%)	31 (9%)	9 (3%)	7 10
2	M	350/352 (99%)	320 (91%)	19 (5%)	11 (3%)	5 7
3	C	383/385 (100%)	364 (95%)	17 (4%)	2 (0%)	34 55
3	N	383/385 (100%)	367 (96%)	14 (4%)	2 (0%)	34 55
4	D	244/248 (98%)	231 (95%)	12 (5%)	1 (0%)	39 61
4	O	244/248 (98%)	234 (96%)	10 (4%)	0	100 100
5	E	183/185 (99%)	171 (93%)	9 (5%)	3 (2%)	12 21
5	P	183/185 (99%)	171 (93%)	10 (6%)	2 (1%)	17 31
6	F	72/146 (49%)	68 (94%)	4 (6%)	0	100 100
6	Q	72/146 (49%)	67 (93%)	4 (6%)	1 (1%)	14 24
7	G	123/126 (98%)	121 (98%)	2 (2%)	0	100 100
7	R	123/126 (98%)	119 (97%)	4 (3%)	0	100 100
8	H	91/93 (98%)	78 (86%)	10 (11%)	3 (3%)	5 6
8	S	91/93 (98%)	82 (90%)	6 (7%)	3 (3%)	5 6
9	I	53/65 (82%)	48 (91%)	4 (8%)	1 (2%)	10 16
9	T	53/65 (82%)	50 (94%)	1 (2%)	2 (4%)	4 5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
10	J	125/127 (98%)	110 (88%)	14 (11%)	1 (1%)	24 41
10	U	125/127 (98%)	110 (88%)	12 (10%)	3 (2%)	7 11
11	K	105/107 (98%)	80 (76%)	21 (20%)	4 (4%)	4 5
11	V	105/107 (98%)	82 (78%)	20 (19%)	3 (3%)	6 8
12	W	110/112 (98%)	98 (89%)	11 (10%)	1 (1%)	21 37
All	All	4426/4642 (95%)	4069 (92%)	300 (7%)	57 (1%)	15 26

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	152	ARG
2	B	153	LYS
2	B	335	PRO
2	B	343	VAL
3	C	346	VAL
8	H	37	LEU
8	H	93	ASN
11	K	80	PRO
2	M	153	LYS
2	M	335	PRO
2	M	343	VAL
2	M	348	LEU
5	P	103	LEU
2	B	214	SER
2	B	311	GLY
2	B	327	VAL
3	C	223	SER
5	E	102	PRO
5	E	103	LEU
8	H	36	PRO
10	J	65	LYS
1	L	126	GLN
2	M	311	GLY
2	M	338	LEU
3	N	223	SER
6	Q	118	GLU
8	S	37	LEU
2	B	338	LEU
5	E	46	ASN
9	I	55	ARG

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Mol	Chain	Res	Type
11	K	51	THR
1	L	227	ASN
2	M	313	ASP
5	P	102	PRO
9	T	12	LYS
9	T	13	ARG
10	U	44	ASN
11	V	30	ASN
1	L	228	LEU
2	M	95	LYS
8	S	93	ASN
10	U	32	GLY
12	W	6	GLY
1	A	127	GLN
4	D	263	HIS
11	K	10	SER
2	M	315	SER
2	M	327	VAL
8	S	36	PRO
10	U	15	SER
11	K	16	GLY
1	L	231	GLN
2	M	314	LEU
3	N	346	VAL
11	V	68	GLY
2	B	332	VAL
11	V	80	PRO

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	370/370 (100%)	338 (91%)	32 (9%)	13 24
1	L	370/370 (100%)	334 (90%)	36 (10%)	10 19
2	B	301/301 (100%)	273 (91%)	28 (9%)	11 21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	M	301/301 (100%)	274 (91%)	27 (9%)	12 22
3	C	338/338 (100%)	317 (94%)	21 (6%)	23 41
3	N	338/338 (100%)	320 (95%)	18 (5%)	28 50
4	D	204/206 (99%)	197 (97%)	7 (3%)	44 72
4	O	204/206 (99%)	197 (97%)	7 (3%)	44 72
5	E	151/151 (100%)	147 (97%)	4 (3%)	54 81
5	P	151/151 (100%)	147 (97%)	4 (3%)	54 81
6	F	67/130 (52%)	64 (96%)	3 (4%)	34 59
6	Q	67/130 (52%)	64 (96%)	3 (4%)	34 59
7	G	109/110 (99%)	104 (95%)	5 (5%)	33 57
7	R	109/110 (99%)	104 (95%)	5 (5%)	33 57
8	H	77/77 (100%)	76 (99%)	1 (1%)	76 92
8	S	77/77 (100%)	75 (97%)	2 (3%)	54 81
9	I	45/53 (85%)	44 (98%)	1 (2%)	60 84
9	T	45/53 (85%)	43 (96%)	2 (4%)	35 60
10	J	112/112 (100%)	105 (94%)	7 (6%)	22 40
10	U	112/112 (100%)	102 (91%)	10 (9%)	12 23
11	K	93/93 (100%)	86 (92%)	7 (8%)	17 31
11	V	93/93 (100%)	88 (95%)	5 (5%)	27 49
12	W	92/91 (101%)	86 (94%)	6 (6%)	21 39
All	All	3826/3973 (96%)	3585 (94%)	241 (6%)	22 40

All (241) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	ASN
1	A	113	THR
1	A	115	LYS
1	A	126	GLN
1	A	164	LEU
1	A	172	THR
1	A	179	ARG
1	A	185	LEU
1	A	188	LEU
1	A	193	LEU

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Mol	Chain	Res	Type
1	A	203	ASN
1	A	239	LYS
1	A	252	ARG
1	A	261	ILE
1	A	271	ASN
1	A	272	SER
1	A	289	ASN
1	A	311	LEU
1	A	320	LEU
1	A	330	PHE
1	A	336	ASN
1	A	343	LEU
1	A	361	THR
1	A	370	LEU
1	A	377	LEU
1	A	384	VAL
1	A	390	LEU
1	A	425	ARG
1	A	426	LEU
1	A	429	GLN
1	A	443	LEU
1	A	456	ARG
2	B	30	THR
2	B	31	LEU
2	B	53	ARG
2	B	54	PHE
2	B	62	ARG
2	B	73	LEU
2	B	128	ARG
2	B	136	GLN
2	B	144	ASP
2	B	146	LEU
2	B	150	THR
2	B	155	LEU
2	B	166	ARG
2	B	169	LEU
2	B	206	LEU
2	B	215	LEU
2	B	250	LEU
2	B	252	GLN
2	B	254	GLU
2	B	255	VAL

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Mol	Chain	Res	Type
2	B	270	LEU
2	B	312	LYS
2	B	323	LEU
2	B	330	GLU
2	B	339	ASN
2	B	343	VAL
2	B	347	LYS
2	B	362	LEU
3	C	38	LEU
3	C	79	ARG
3	C	89	PHE
3	C	99	LYS
3	C	107	ARG
3	C	111	VAL
3	C	150	LEU
3	C	175	THR
3	C	182	LEU
3	C	184	TYR
3	C	185	LEU
3	C	238	LEU
3	C	247	SER
3	C	292	VAL
3	C	302	LEU
3	C	312	VAL
3	C	313	VAL
3	C	336	LEU
3	C	350	LEU
3	C	377	LEU
3	C	382	ARG
4	D	113	ARG
4	D	141	GLN
4	D	147	ARG
4	D	251	VAL
4	D	256	ASN
4	D	280	LEU
4	D	288	LYS
5	E	114	LYS
5	E	208	ASP
5	E	211	LYS
5	E	213	ILE
6	F	77	GLN
6	F	94	LEU

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Mol	Chain	Res	Type
6	F	130	LEU
7	G	16	LEU
7	G	58	THR
7	G	97	GLN
7	G	123	ILE
7	G	127	LYS
8	H	60	LEU
9	I	18	VAL
10	J	38	ILE
10	J	39	ARG
10	J	44	ASN
10	J	51	TYR
10	J	61	ASN
10	J	68	LEU
10	J	114	GLN
11	K	7	THR
11	K	18	ARG
11	K	33	LEU
11	K	77	ASN
11	K	81	GLU
11	K	92	ILE
11	K	93	LYS
1	L	30	THR
1	L	66	ASN
1	L	89	GLU
1	L	117	LEU
1	L	120	LEU
1	L	126	GLN
1	L	130	ASN
1	L	153	ASP
1	L	164	LEU
1	L	172	THR
1	L	174	LEU
1	L	176	LEU
1	L	179	ARG
1	L	185	LEU
1	L	188	LEU
1	L	218	ASP
1	L	237	VAL
1	L	238	LEU
1	L	239	LYS
1	L	241	LYS

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Mol	Chain	Res	Type
1	L	261	ILE
1	L	289	ASN
1	L	293	PRO
1	L	311	LEU
1	L	320	LEU
1	L	330	PHE
1	L	336	ASN
1	L	343	LEU
1	L	370	LEU
1	L	374	LEU
1	L	377	LEU
1	L	390	LEU
1	L	424	LYS
1	L	425	ARG
1	L	426	LEU
1	L	443	LEU
2	M	17	LEU
2	M	30	THR
2	M	31	LEU
2	M	40	ARG
2	M	53	ARG
2	M	54	PHE
2	M	62	ARG
2	M	73	LEU
2	M	111	LYS
2	M	136	GLN
2	M	144	ASP
2	M	146	LEU
2	M	166	ARG
2	M	169	LEU
2	M	186	GLU
2	M	206	LEU
2	M	238	VAL
2	M	246	ASN
2	M	250	LEU
2	M	255	VAL
2	M	310	LYS
2	M	312	LYS
2	M	329	ASN
2	M	330	GLU
2	M	345	ASP
2	M	347	LYS

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Mol	Chain	Res	Type
2	M	362	LEU
3	N	35	LEU
3	N	38	LEU
3	N	79	ARG
3	N	87	SER
3	N	89	PHE
3	N	99	LYS
3	N	150	LEU
3	N	182	LEU
3	N	184	TYR
3	N	185	LEU
3	N	208	ASN
3	N	218	ARG
3	N	302	LEU
3	N	312	VAL
3	N	336	LEU
3	N	350	LEU
3	N	377	LEU
3	N	382	ARG
4	O	69	LEU
4	O	163	GLN
4	O	179	LEU
4	O	251	VAL
4	O	256	ASN
4	O	280	LEU
4	O	283	LEU
5	P	51	LYS
5	P	65	LEU
5	P	80	SER
5	P	211	LYS
6	Q	77	GLN
6	Q	94	LEU
6	Q	130	LEU
7	R	16	LEU
7	R	41	LEU
7	R	97	GLN
7	R	125	VAL
7	R	127	LYS
8	S	50	ARG
8	S	68	TYR
9	T	14	ASN
9	T	18	VAL

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Mol	Chain	Res	Type
10	U	3	LYS
10	U	21	THR
10	U	38	ILE
10	U	39	ARG
10	U	51	TYR
10	U	54	ASN
10	U	59	ASN
10	U	61	ASN
10	U	66	ASP
10	U	68	LEU
11	V	18	ARG
11	V	41	ASP
11	V	81	GLU
11	V	89	GLN
11	V	92	ILE
12	W	2	LYS
12	W	20	LYS
12	W	51	GLN
12	W	58	THR
12	W	82	LYS
12	W	98	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (136) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	ASN
1	A	66	ASN
1	A	67	ASN
1	A	96	ASN
1	A	102	GLN
1	A	130	ASN
1	A	156	HIS
1	A	199	ASN
1	A	231	GLN
1	A	271	ASN
1	A	274	ASN
1	A	289	ASN
1	A	317	HIS
1	A	336	ASN
1	A	350	GLN
1	A	382	ASN
1	A	385	ASN

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Mol	Chain	Res	Type
1	A	388	ASN
1	A	429	GLN
2	B	49	HIS
2	B	52	ASN
2	B	55	ASN
2	B	57	GLN
2	B	103	ASN
2	B	191	ASN
2	B	246	ASN
2	B	252	GLN
2	B	258	ASN
2	B	339	ASN
3	C	14	ASN
3	C	22	GLN
3	C	74	ASN
3	C	173	ASN
3	C	202	HIS
3	C	208	ASN
3	C	253	HIS
3	C	332	ASN
4	D	78	HIS
4	D	79	ASN
4	D	127	ASN
4	D	141	GLN
4	D	256	ASN
5	E	38	ASN
5	E	47	ASN
5	E	106	ASN
5	E	184	HIS
6	F	77	GLN
6	F	84	HIS
6	F	108	GLN
6	F	109	GLN
6	F	111	GLN
6	F	129	HIS
7	G	30	ASN
7	G	53	ASN
7	G	79	HIS
7	G	91	ASN
7	G	97	GLN
8	H	55	GLN
8	H	74	ASN

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Mol	Chain	Res	Type
9	I	14	ASN
9	I	29	GLN
10	J	44	ASN
10	J	54	ASN
10	J	61	ASN
10	J	77	ASN
10	J	78	GLN
11	K	34	ASN
11	K	89	GLN
11	K	91	HIS
1	L	61	ASN
1	L	66	ASN
1	L	67	ASN
1	L	102	GLN
1	L	127	GLN
1	L	130	ASN
1	L	156	HIS
1	L	170	GLN
1	L	199	ASN
1	L	227	ASN
1	L	274	ASN
1	L	283	GLN
1	L	289	ASN
1	L	317	HIS
1	L	336	ASN
1	L	350	GLN
1	L	385	ASN
1	L	388	ASN
1	L	438	GLN
2	M	49	HIS
2	M	52	ASN
2	M	55	ASN
2	M	246	ASN
2	M	252	GLN
2	M	329	ASN
2	M	339	ASN
3	N	14	ASN
3	N	22	GLN
3	N	43	GLN
3	N	74	ASN
3	N	208	ASN
3	N	253	HIS

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Mol	Chain	Res	Type
3	N	332	ASN
4	O	78	HIS
4	O	79	ASN
4	O	127	ASN
4	O	163	GLN
4	O	256	ASN
5	P	38	ASN
5	P	97	ASN
5	P	106	ASN
5	P	112	GLN
5	P	184	HIS
6	Q	77	GLN
7	R	30	ASN
7	R	31	GLN
7	R	53	ASN
7	R	57	GLN
7	R	79	HIS
7	R	91	ASN
7	R	97	GLN
8	S	38	GLN
8	S	55	GLN
9	T	14	ASN
9	T	29	GLN
10	U	54	ASN
10	U	58	ASN
10	U	59	ASN
10	U	61	ASN
10	U	77	ASN
10	U	78	GLN
11	V	34	ASN
11	V	90	HIS
11	V	91	HIS
12	W	25	GLN
12	W	61	ASN
12	W	101	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\#\|Z\| > 2$
12	M3L	W	81	12	10,11,12	0.82	0	12,14,16	1.19	1 (8%)

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
12	M3L	W	81	12	-	0/8/10/12	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	W	81	M3L	CM3-NZ-CM1	-2.54	102.43	108.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

24 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	$\#\|Z\| > 2$
14	UMQ	A	4021	-	35,35,35	0.96	1 (2%)	46,46,46	1.69	7 (15%)
15	HEM	C	4001	3	30,50,50	3.14	11 (36%)	24,82,82	1.92	6 (25%)
15	HEM	C	4002	3	30,50,50	2.80	9 (30%)	24,82,82	2.29	8 (33%)
16	SMA	C	4005	-	35,38,38	1.33	4 (11%)	40,52,52	1.51	6 (15%)
17	8PE	C	4010	-	45,46,46	0.94	3 (6%)	46,51,51	1.03	1 (2%)
18	CN6	C	4031	-	49,49,49	1.54	11 (22%)	51,61,61	1.45	5 (9%)
19	9PE	C	4111	-	38,39,39	0.73	0	39,44,44	0.96	1 (2%)
15	HEM	D	4003	4	30,50,50	2.62	7 (23%)	24,82,82	3.23	8 (33%)
20	7PH	D	4014	-	37,37,37	1.02	2 (5%)	40,42,42	1.47	9 (22%)
21	FES	E	4004	5	0,4,4	0.00	-	0,4,4	0.00	-
22	6PH	E	4013	-	39,39,39	0.95	2 (5%)	42,44,44	1.34	4 (9%)
22	6PH	L	4113	-	39,39,39	0.98	2 (5%)	42,44,44	1.37	4 (9%)
14	UMQ	L	4121	-	35,35,35	0.98	1 (2%)	46,46,46	1.75	5 (10%)
19	9PE	N	4011	-	38,39,39	0.69	0	39,44,44	0.91	1 (2%)
15	HEM	N	4021	3	30,50,50	3.10	11 (36%)	24,82,82	2.24	8 (33%)
15	HEM	N	4022	3	30,50,50	2.98	12 (40%)	24,82,82	2.60	8 (33%)
16	SMA	N	4025	-	35,38,38	1.29	2 (5%)	40,52,52	1.38	4 (10%)
17	8PE	N	4110	-	45,46,46	0.90	2 (4%)	46,51,51	1.21	3 (6%)
18	CN6	N	4131	-	49,49,49	1.59	10 (20%)	51,61,61	1.60	6 (11%)
15	HEM	O	4023	4	30,50,50	2.54	8 (26%)	24,82,82	3.17	10 (41%)
20	7PH	O	4114	-	37,37,37	1.04	2 (5%)	40,42,42	1.51	9 (22%)
13	SUC	O	4146	-	24,24,24	0.62	0	36,36,36	0.68	1 (2%)
21	FES	P	4024	5	0,4,4	0.00	-	0,4,4	0.00	-
15	HEM	W	4026	12	30,50,50	2.65	9 (30%)	24,82,82	3.07	9 (37%)

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
14	UMQ	A	4021	-	-	0/20/60/60	0/2/2/2
15	HEM	C	4001	3	-	0/10/54/54	0/0/8/8
15	HEM	C	4002	3	-	0/10/54/54	0/0/8/8
16	SMA	C	4005	-	-	0/33/34/34	0/2/2/2
17	8PE	C	4010	-	-	0/50/50/50	0/0/0/0
18	CN6	C	4031	-	-	1/60/60/60	0/0/0/0
19	9PE	C	4111	-	-	0/43/43/43	0/0/0/0
15	HEM	D	4003	4	-	0/10/54/54	0/0/8/8
20	7PH	D	4014	-	-	0/39/39/39	0/0/0/0
21	FES	E	4004	5	-	0/0/4/4	0/1/1/1
22	6PH	E	4013	-	-	0/41/41/41	0/0/0/0
22	6PH	L	4113	-	-	0/41/41/41	0/0/0/0
14	UMQ	L	4121	-	-	0/20/60/60	0/2/2/2
19	9PE	N	4011	-	-	0/43/43/43	0/0/0/0
15	HEM	N	4021	3	-	0/10/54/54	0/0/8/8
15	HEM	N	4022	3	-	0/10/54/54	0/0/8/8
16	SMA	N	4025	-	-	0/33/34/34	0/2/2/2
17	8PE	N	4110	-	-	0/50/50/50	0/0/0/0
18	CN6	N	4131	-	-	0/60/60/60	0/0/0/0
15	HEM	O	4023	4	-	0/10/54/54	0/0/8/8
20	7PH	O	4114	-	-	0/39/39/39	0/0/0/0
13	SUC	O	4146	-	-	0/12/51/51	0/2/2/2
21	FES	P	4024	5	-	0/0/4/4	0/1/1/1
15	HEM	W	4026	12	-	0/10/54/54	0/0/8/8

All (109) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	N	4021	HEM	C3B-C4B	-8.39	1.44	1.51
15	C	4001	HEM	C3B-C4B	-7.87	1.44	1.51
15	D	4003	HEM	C3B-C4B	-7.67	1.45	1.51
15	W	4026	HEM	C3B-C4B	-7.61	1.45	1.51
15	N	4022	HEM	C3B-C4B	-7.32	1.45	1.51
15	O	4023	HEM	C3B-C4B	-7.19	1.45	1.51
15	N	4021	HEM	C3C-CAC	-7.11	1.38	1.51
15	C	4001	HEM	C3C-CAC	-7.08	1.38	1.51
15	C	4001	HEM	C3B-CAB	-7.02	1.38	1.51
15	C	4002	HEM	C3B-C4B	-7.01	1.45	1.51
15	N	4021	HEM	C3B-CAB	-6.69	1.38	1.51
15	N	4021	HEM	C2D-C3D	-6.47	1.35	1.54
15	D	4003	HEM	C2D-C3D	-6.42	1.35	1.54
15	N	4022	HEM	C3B-CAB	-6.37	1.39	1.51
15	C	4002	HEM	C2D-C3D	-6.29	1.35	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	C	4001	HEM	C2D-C3D	-6.28	1.35	1.54
15	N	4022	HEM	C2D-C3D	-6.27	1.35	1.54
15	O	4023	HEM	C2D-C3D	-6.18	1.36	1.54
15	W	4026	HEM	C2D-C3D	-6.14	1.36	1.54
15	C	4001	HEM	C3D-C4D	-5.94	1.43	1.51
15	C	4002	HEM	C3B-CAB	-5.92	1.40	1.51
15	W	4026	HEM	C3D-C4D	-5.75	1.44	1.51
15	N	4022	HEM	C3D-C4D	-5.68	1.44	1.51
15	N	4021	HEM	C3D-C4D	-5.41	1.44	1.51
15	D	4003	HEM	C3D-C4D	-5.33	1.44	1.51
15	C	4002	HEM	C3C-CAC	-5.26	1.41	1.51
15	N	4022	HEM	C3C-CAC	-5.25	1.41	1.51
15	C	4002	HEM	C3D-C4D	-5.09	1.45	1.51
15	O	4023	HEM	C3D-C4D	-4.84	1.45	1.51
18	N	4131	CN6	O31-C3	-4.32	1.35	1.45
18	C	4031	CN6	O31-C3	-4.25	1.35	1.45
15	O	4023	HEM	C2C-C1C	-4.14	1.44	1.52
15	C	4002	HEM	C2C-C1C	-4.08	1.44	1.52
15	D	4003	HEM	C2C-C1C	-4.03	1.44	1.52
15	N	4021	HEM	C2C-C1C	-3.98	1.45	1.52
14	L	4121	UMQ	C3-C2	-3.96	1.42	1.52
15	C	4001	HEM	C2C-C1C	-3.95	1.45	1.52
15	W	4026	HEM	C2C-C1C	-3.94	1.45	1.52
15	N	4022	HEM	C2C-C1C	-3.91	1.45	1.52
20	D	4014	7PH	O31-C3	-3.65	1.36	1.45
20	O	4114	7PH	O31-C3	-3.65	1.36	1.45
18	N	4131	CN6	O21-C2	-3.52	1.37	1.46
14	A	4021	UMQ	C3-C2	-3.50	1.43	1.52
18	C	4031	CN6	O21-C2	-3.49	1.37	1.46
18	C	4031	CN6	O3'-CA	-3.24	1.31	1.44
18	N	4131	CN6	O3'-CA	-3.18	1.31	1.44
18	N	4131	CN6	O32-C31	-3.04	1.13	1.22
18	C	4031	CN6	O32-C31	-2.87	1.14	1.22
17	C	4010	8PE	O32-C31	-2.53	1.15	1.22
15	C	4001	HEM	C2B-C1B	-2.50	1.43	1.51
17	N	4110	8PE	O32-C31	-2.49	1.15	1.22
15	N	4022	HEM	C2D-C1D	-2.48	1.43	1.51
15	N	4021	HEM	C2B-C1B	-2.42	1.43	1.51
18	N	4131	CN6	O11-C1	-2.39	1.35	1.44
18	C	4031	CN6	O11-C1	-2.35	1.35	1.44
15	N	4022	HEM	C2B-C1B	-2.34	1.44	1.51
20	O	4114	7PH	O22-C21	-2.34	1.15	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	C	4001	HEM	C2D-C1D	-2.33	1.44	1.51
15	W	4026	HEM	C2D-C1D	-2.24	1.44	1.51
15	N	4021	HEM	C2D-C1D	-2.24	1.44	1.51
15	C	4002	HEM	C2D-C1D	-2.22	1.44	1.51
15	O	4023	HEM	C2B-C1B	-2.21	1.44	1.51
15	D	4003	HEM	C2B-C1B	-2.19	1.44	1.51
18	N	4131	CN6	O41-C3'	-2.18	1.40	1.45
20	D	4014	7PH	O22-C21	-2.13	1.16	1.22
15	W	4026	HEM	C2B-C1B	-2.10	1.45	1.51
15	O	4023	HEM	C2D-C1D	-2.08	1.45	1.51
18	C	4031	CN6	O41-C3'	-2.06	1.40	1.45
15	W	4026	HEM	C1C-NC	2.04	1.38	1.36
18	C	4031	CN6	O21-C21	2.04	1.40	1.34
15	C	4001	HEM	CBB-CAB	2.06	1.41	1.29
16	C	4005	SMA	C7-C8	2.06	1.43	1.40
15	N	4021	HEM	C1C-NC	2.08	1.38	1.36
18	N	4131	CN6	O21-C21	2.10	1.40	1.34
18	C	4031	CN6	C1'-C2'	2.12	1.56	1.50
16	C	4005	SMA	C4-C3	2.20	1.47	1.41
18	C	4031	CN6	CA-CB	2.21	1.60	1.51
18	C	4031	CN6	OA-CB	2.25	1.50	1.43
22	E	4013	6PH	C1-C2	2.27	1.57	1.50
22	E	4013	6PH	C3-C2	2.28	1.57	1.50
17	C	4010	8PE	C3-C2	2.28	1.57	1.50
15	N	4021	HEM	CBC-CAC	2.28	1.42	1.29
18	N	4131	CN6	CC-CB	2.30	1.60	1.51
15	N	4022	HEM	CBB-CAB	2.35	1.42	1.29
22	L	4113	6PH	C3-C2	2.36	1.57	1.50
18	N	4131	CN6	OA-CB	2.36	1.50	1.43
15	C	4001	HEM	CBC-CAC	2.40	1.43	1.29
17	N	4110	8PE	O21-C21	2.44	1.41	1.34
15	N	4022	HEM	C1C-NC	2.51	1.39	1.36
22	L	4113	6PH	C1-C2	2.52	1.57	1.50
18	C	4031	CN6	CC-CB	2.52	1.61	1.51
15	C	4001	HEM	C1C-NC	2.52	1.39	1.36
18	N	4131	CN6	CA-CB	2.61	1.61	1.51
15	N	4021	HEM	CBB-CAB	2.62	1.44	1.29
15	C	4002	HEM	CBB-CAB	2.83	1.45	1.29
17	C	4010	8PE	O21-C21	2.83	1.42	1.34
15	C	4002	HEM	CBC-CAC	3.09	1.47	1.29
15	N	4022	HEM	CMA-C3A	3.23	1.58	1.51
15	N	4022	HEM	CBC-CAC	3.35	1.48	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	W	4026	HEM	CBB-CAB	3.98	1.52	1.29
15	O	4023	HEM	CBC-CAC	4.02	1.52	1.29
15	D	4003	HEM	CBB-CAB	4.13	1.53	1.29
15	W	4026	HEM	CBC-CAC	4.17	1.53	1.29
16	N	4025	SMA	O1-C2	4.21	1.40	1.35
15	D	4003	HEM	CBC-CAC	4.23	1.53	1.29
16	C	4005	SMA	O1-C2	4.34	1.40	1.35
15	O	4023	HEM	CBB-CAB	4.35	1.54	1.29
16	N	4025	SMA	C4-C4A	4.45	1.47	1.41
16	C	4005	SMA	C4-C4A	4.45	1.47	1.41

All (123) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	D	4003	HEM	C3B-CAB-CBB	-9.56	109.79	124.46
15	O	4023	HEM	C3B-CAB-CBB	-9.40	110.04	124.46
15	D	4003	HEM	C3C-CAC-CBC	-8.55	111.34	124.46
14	L	4121	UMQ	CA-O1'-C1'	-8.36	99.33	113.94
15	W	4026	HEM	C3B-CAB-CBB	-7.99	112.19	124.46
15	W	4026	HEM	C3C-CAC-CBC	-7.77	112.53	124.46
14	A	4021	UMQ	CA-O1'-C1'	-7.75	100.40	113.94
15	O	4023	HEM	C3C-CAC-CBC	-6.31	114.77	124.46
18	N	4131	CN6	C2'-O51-C51	-5.68	104.25	117.89
16	C	4005	SMA	C3-C4-C4A	-4.56	115.02	121.35
22	L	4113	6PH	C3-C2-C1	-4.55	101.42	112.07
22	E	4013	6PH	C3-C2-C1	-4.38	101.83	112.07
18	C	4031	CN6	C2'-O51-C51	-4.35	107.45	117.89
16	N	4025	SMA	C3-C4-C4A	-4.31	115.37	121.35
18	N	4131	CN6	C2-O21-C21	-4.11	108.04	117.89
18	C	4031	CN6	C2-O21-C21	-4.04	108.20	117.89
18	N	4131	CN6	C3'-C2'-C1'	-3.91	102.93	112.07
18	C	4031	CN6	C3-C2-C1	-3.78	103.22	112.07
19	C	4111	9PE	C2-O21-C21	-3.72	108.95	117.89
18	N	4131	CN6	C3-C2-C1	-3.67	103.48	112.07
20	D	4014	7PH	C38-C37-C36	-3.59	96.01	114.53
17	N	4110	8PE	C2-O21-C21	-3.54	109.39	117.89
20	O	4114	7PH	C38-C37-C36	-3.41	96.92	114.53
16	C	4005	SMA	C9-C10-C11	-3.38	110.77	114.75
15	N	4021	HEM	CBA-CAA-C2A	-3.30	106.61	112.53
17	C	4010	8PE	C2-O21-C21	-3.21	110.20	117.89
15	N	4021	HEM	CAA-C2A-C1A	-3.20	123.54	127.01
19	N	4011	9PE	C2-O21-C21	-3.17	110.29	117.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	D	4014	7PH	C3-C2-C1	-3.07	104.90	112.07
20	O	4114	7PH	O31-C3-C2	-3.02	100.55	108.69
20	O	4114	7PH	O11-P-O14	-2.97	99.59	107.14
16	N	4025	SMA	C9-C10-C11	-2.87	111.37	114.75
13	O	4146	SUC	C4-C3-C2	-2.75	105.66	110.79
17	N	4110	8PE	O31-C3-C2	-2.74	101.31	108.69
20	D	4014	7PH	O11-P-O14	-2.73	100.18	107.14
18	C	4031	CN6	C3'-C2'-C1'	-2.71	105.74	112.07
20	O	4114	7PH	C3-C2-C1	-2.64	105.89	112.07
15	N	4022	HEM	CAA-C2A-C1A	-2.58	124.21	127.01
20	D	4014	7PH	O12-P-O14	-2.55	102.38	110.58
22	L	4113	6PH	O14-P-O11	-2.47	99.44	106.56
20	O	4114	7PH	O31-C31-C32	-2.47	104.39	111.90
20	O	4114	7PH	O12-P-O14	-2.46	102.67	110.58
14	A	4021	UMQ	C3'-C4'-C5'	-2.40	105.41	110.84
14	A	4021	UMQ	CD-CC-CB	-2.38	102.25	114.53
14	L	4121	UMQ	C3'-C4'-C5'	-2.38	105.46	110.84
20	D	4014	7PH	O31-C3-C2	-2.36	102.34	108.69
22	E	4013	6PH	O14-P-O11	-2.36	99.78	106.56
14	L	4121	UMQ	CD-CC-CB	-2.31	102.58	114.53
15	W	4026	HEM	CBD-CAD-C3D	-2.30	106.86	113.55
20	D	4014	7PH	O31-C31-C32	-2.29	104.92	111.90
14	A	4021	UMQ	O1-C1-O5	-2.22	105.05	110.68
15	O	4023	HEM	CAA-C2A-C3A	-2.17	122.82	129.00
14	A	4021	UMQ	C1-O5-C5	-2.04	109.78	113.75
16	C	4005	SMA	O1-C8A-C4A	2.04	123.26	121.15
15	D	4003	HEM	CMD-C2D-C3D	2.05	123.40	114.35
20	O	4114	7PH	O31-C31-O32	2.17	129.10	123.49
20	D	4014	7PH	O31-C31-O32	2.19	129.15	123.49
16	N	4025	SMA	C4-C3-C2	2.19	120.92	117.73
18	N	4131	CN6	OA-CB-CA	2.22	117.82	109.35
15	C	4002	HEM	C3C-CAC-CBC	2.24	127.90	124.46
16	C	4005	SMA	O8-C8-C7	2.29	124.38	119.34
20	D	4014	7PH	O13-P-O11	2.36	113.37	106.56
14	A	4021	UMQ	O1'-C1'-C2'	2.40	111.07	108.04
16	C	4005	SMA	C4-C3-C2	2.40	121.22	117.73
18	C	4031	CN6	O3'-P'-O4'	2.56	119.57	109.62
20	O	4114	7PH	O13-P-O11	2.60	114.06	106.56
18	N	4131	CN6	O3'-P'-O4'	2.64	119.86	109.62
22	E	4013	6PH	O13-P-O11	2.74	114.44	106.56
14	L	4121	UMQ	O1'-C1'-C2'	2.75	111.52	108.04
15	O	4023	HEM	CAA-C2A-C1A	2.80	130.04	127.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	C	4001	HEM	CMC-C2C-C3C	2.87	123.70	116.53
15	N	4021	HEM	CMD-C2D-C3D	2.88	127.09	114.35
15	W	4026	HEM	CMD-C2D-C3D	2.92	127.28	114.35
22	L	4113	6PH	O13-P-O11	2.93	115.00	106.56
15	N	4021	HEM	CAD-C3D-C2D	2.93	121.65	113.22
15	N	4021	HEM	C2D-C3D-C4D	2.97	106.53	101.50
14	L	4121	UMQ	O1'-CA-CB	3.01	121.84	109.88
15	O	4023	HEM	CMD-C2D-C3D	3.04	127.80	114.35
15	C	4001	HEM	CMD-C2D-C3D	3.07	127.93	114.35
15	O	4023	HEM	C2D-C3D-C4D	3.09	106.74	101.50
15	C	4002	HEM	C2D-C3D-C4D	3.12	106.78	101.50
15	D	4003	HEM	C2D-C3D-C4D	3.15	106.85	101.50
15	C	4001	HEM	C2D-C3D-C4D	3.16	106.86	101.50
15	N	4022	HEM	CMD-C2D-C3D	3.21	128.56	114.35
14	A	4021	UMQ	O1'-CA-CB	3.23	122.74	109.88
15	N	4022	HEM	C2D-C3D-C4D	3.25	107.02	101.50
20	D	4014	7PH	O12-P-O11	3.31	116.08	106.56
17	N	4110	8PE	C3-C2-C1	3.32	119.83	112.07
15	C	4002	HEM	C3B-CAB-CBB	3.32	129.55	124.46
15	W	4026	HEM	C2D-C3D-C4D	3.34	107.17	101.50
15	D	4003	HEM	CMC-C2C-C3C	3.42	125.06	116.53
15	D	4003	HEM	CAD-C3D-C2D	3.43	123.06	113.22
15	C	4002	HEM	CMD-C2D-C3D	3.46	129.64	114.35
20	O	4114	7PH	O12-P-O11	3.52	116.70	106.56
15	N	4021	HEM	CMC-C2C-C3C	3.63	125.60	116.53
15	O	4023	HEM	CAD-C3D-C2D	3.70	123.86	113.22
15	W	4026	HEM	CMC-C2C-C3C	3.72	125.81	116.53
22	L	4113	6PH	O11-P-O12	3.72	116.61	107.14
22	E	4013	6PH	O11-P-O12	3.77	116.73	107.14
15	O	4023	HEM	CMC-C2C-C3C	3.98	126.48	116.53
15	W	4026	HEM	CAD-C3D-C4D	4.05	126.76	112.47
15	C	4001	HEM	CMB-C2B-C3B	4.05	126.65	116.53
15	D	4003	HEM	CMB-C2B-C3B	4.05	126.65	116.53
15	N	4022	HEM	CAD-C3D-C4D	4.06	126.78	112.47
15	W	4026	HEM	CMB-C2B-C3B	4.07	126.69	116.53
15	C	4002	HEM	CAD-C3D-C4D	4.09	126.88	112.47
15	C	4001	HEM	CAD-C3D-C2D	4.10	125.00	113.22
15	O	4023	HEM	CMB-C2B-C3B	4.15	126.89	116.53
15	W	4026	HEM	CAD-C3D-C2D	4.42	125.93	113.22
15	C	4001	HEM	CAD-C3D-C4D	4.44	128.13	112.47
15	N	4022	HEM	CAD-C3D-C2D	4.50	126.15	113.22
15	C	4002	HEM	CAD-C3D-C2D	4.53	126.25	113.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	C	4002	HEM	CMB-C2B-C3B	4.58	127.96	116.53
15	N	4022	HEM	CMC-C2C-C3C	4.63	128.09	116.53
16	C	4005	SMA	C9-C2-C3	4.63	126.67	120.56
16	N	4025	SMA	C9-C2-C3	4.69	126.75	120.56
15	O	4023	HEM	CAD-C3D-C4D	4.79	129.36	112.47
15	C	4002	HEM	CMC-C2C-C3C	4.81	128.54	116.53
15	D	4003	HEM	CAD-C3D-C4D	4.99	130.07	112.47
15	N	4022	HEM	C3C-CAC-CBC	5.16	132.37	124.46
15	N	4021	HEM	CMB-C2B-C3B	5.18	129.45	116.53
15	N	4021	HEM	CAD-C3D-C4D	5.39	131.47	112.47
15	N	4022	HEM	CMB-C2B-C3B	5.89	131.23	116.53

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	C	4031	CN6	C2'-O51-C51-C52

There are no ring outliers.

18 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	4021	UMQ	4	0
15	C	4001	HEM	2	0
15	C	4002	HEM	1	0
16	C	4005	SMA	1	0
17	C	4010	8PE	2	0
18	C	4031	CN6	7	0
20	D	4014	7PH	3	0
22	E	4013	6PH	1	0
14	L	4121	UMQ	2	0
15	N	4022	HEM	1	0
16	N	4025	SMA	1	0
17	N	4110	8PE	2	0
18	N	4131	CN6	5	0
15	O	4023	HEM	1	0
20	O	4114	7PH	2	0
13	O	4146	SUC	2	0
21	P	4024	FES	1	0
15	W	4026	HEM	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	431/431 (100%)	0.41	40 (9%) 11 11	32, 57, 121, 146	0
1	L	431/431 (100%)	0.34	41 (9%) 10 11	29, 53, 114, 140	0
2	B	352/352 (100%)	0.55	32 (9%) 11 12	40, 61, 101, 148	0
2	M	352/352 (100%)	0.51	31 (8%) 12 13	40, 59, 93, 137	0
3	C	385/385 (100%)	-0.30	6 (1%) 74 78	26, 35, 49, 113	0
3	N	385/385 (100%)	-0.26	6 (1%) 74 78	25, 33, 46, 104	0
4	D	246/248 (99%)	0.01	11 (4%) 37 42	32, 48, 70, 79	0
4	O	246/248 (99%)	-0.14	5 (2%) 68 72	25, 42, 64, 80	0
5	E	185/185 (100%)	0.54	21 (11%) 7 6	32, 54, 90, 117	0
5	P	185/185 (100%)	0.44	18 (9%) 10 10	34, 52, 92, 114	0
6	F	74/146 (50%)	0.86	13 (17%) 2 2	44, 62, 112, 114	0
6	Q	74/146 (50%)	0.48	12 (16%) 3 2	39, 57, 108, 110	0
7	G	125/126 (99%)	0.02	4 (3%) 51 56	32, 45, 72, 92	0
7	R	125/126 (99%)	0.00	6 (4%) 34 39	28, 43, 69, 88	0
8	H	93/93 (100%)	1.16	20 (21%) 1 1	29, 57, 147, 154	0
8	S	93/93 (100%)	1.42	23 (24%) 1 1	26, 55, 154, 160	0
9	I	55/65 (84%)	0.65	8 (14%) 3 3	41, 56, 111, 124	0
9	T	55/65 (84%)	0.58	8 (14%) 3 3	37, 49, 112, 124	0
10	J	127/127 (100%)	1.03	20 (15%) 3 2	50, 74, 93, 99	0
10	U	127/127 (100%)	0.99	21 (16%) 2 2	52, 74, 89, 97	0
11	K	107/107 (100%)	1.98	48 (44%) 0 0	70, 105, 135, 141	0
11	V	107/107 (100%)	2.01	42 (39%) 0 0	72, 104, 133, 136	0
12	W	111/112 (99%)	1.23	24 (21%) 1 1	50, 70, 108, 136	0
All	All	4471/4642 (96%)	0.42	460 (10%) 9 9	25, 53, 111, 160	0

All (460) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
8	S	43	ASN	15.5
12	W	4	SER	12.8
8	S	42	HIS	11.5
9	T	58	ALA	11.5
8	S	46	PHE	11.1
8	H	43	ASN	10.5
8	S	40	ILE	10.3
1	A	27	ALA	10.2
1	L	27	ALA	9.7
2	B	331	SER	9.1
12	W	5	THR	9.1
3	N	384	ASN	8.8
8	H	42	HIS	8.8
8	S	45	VAL	8.7
12	W	3	GLU	8.5
1	A	231	GLN	8.3
12	W	1	ALA	8.0
1	A	228	LEU	7.9
8	H	41	PHE	7.9
11	V	80	PRO	7.8
5	E	47	ASN	7.7
9	I	58	ALA	7.5
5	E	46	ASN	7.4
5	P	47	ASN	7.2
8	H	46	PHE	7.0
2	B	333	SER	6.9
8	S	50	ARG	6.8
9	T	57	ALA	6.8
2	B	336	ILE	6.8
3	C	385	LYS	6.7
8	S	41	PHE	6.7
12	W	2	LYS	6.5
2	B	332	VAL	6.5
8	H	94	VAL	6.5
2	M	338	LEU	6.4
11	V	106	ILE	6.4
1	A	229	SER	6.3
1	L	127	GLN	6.3
2	B	338	LEU	6.3
1	L	128	LYS	6.3
1	A	230	LEU	6.2
8	S	52	PHE	6.2

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Mol	Chain	Res	Type	RSRZ
9	I	57	ALA	6.2
2	M	311	GLY	6.1
1	A	29	VAL	6.1
5	E	100	ALA	6.0
2	B	330	GLU	6.0
8	H	44	ALA	6.0
2	M	330	GLU	5.9
6	F	112	PRO	5.8
1	L	129	ALA	5.8
6	Q	118	GLU	5.8
3	N	385	LYS	5.8
3	C	384	ASN	5.7
1	L	228	LEU	5.7
11	V	30	ASN	5.6
8	H	49	PHE	5.6
8	S	44	ALA	5.5
8	H	47	ASN	5.5
1	A	28	GLU	5.5
1	L	230	LEU	5.5
6	Q	119	HIS	5.5
1	L	28	GLU	5.4
8	H	50	ARG	5.3
10	J	65	LYS	5.3
6	F	113	GLY	5.2
10	U	42	PRO	5.2
8	H	38	GLN	5.1
1	A	234	THR	5.1
5	P	46	ASN	5.1
2	M	336	ILE	5.1
8	H	39	GLY	5.1
8	S	2	GLY	5.1
5	E	153	LEU	5.0
7	R	127	LYS	5.0
8	S	94	VAL	5.0
1	A	126	GLN	5.0
11	K	86	TYR	5.0
8	S	49	PHE	5.0
11	K	15	LEU	4.9
1	L	234	THR	4.9
1	L	231	GLN	4.9
8	H	5	SER	4.8
12	W	112	LYS	4.8

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Mol	Chain	Res	Type	RSRZ
8	S	47	ASN	4.8
1	L	126	GLN	4.8
5	P	209	GLY	4.7
2	M	331	SER	4.7
11	K	8	PRO	4.7
11	K	75	ILE	4.7
1	L	29	VAL	4.6
5	P	153	LEU	4.6
11	V	79	GLU	4.6
1	A	127	GLN	4.6
6	F	119	HIS	4.6
5	E	210	ASP	4.5
10	J	62	PRO	4.5
1	A	457	TRP	4.5
1	A	233	GLY	4.5
4	D	239	GLY	4.5
11	V	18	ARG	4.5
8	S	48	SER	4.5
9	I	56	ILE	4.5
1	A	238	LEU	4.5
11	K	16	GLY	4.5
11	V	29	ILE	4.5
8	S	68	TYR	4.4
3	N	383	VAL	4.4
11	V	24	ARG	4.4
10	U	1	GLU	4.4
10	J	55	VAL	4.4
1	L	42	HIS	4.4
8	S	39	GLY	4.4
6	F	116	ASP	4.3
1	L	229	SER	4.3
1	L	217	GLU	4.3
2	M	333	SER	4.3
11	K	107	LYS	4.3
2	B	343	VAL	4.3
1	L	31	GLN	4.3
5	P	91	MET	4.2
2	B	240	ALA	4.2
11	V	88	CYS	4.2
6	Q	113	GLY	4.2
10	U	66	ASP	4.2
8	H	40	ILE	4.2

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Mol	Chain	Res	Type	RSRZ
10	U	55	VAL	4.1
10	J	15	SER	4.1
5	P	210	ASP	4.1
11	K	65	SER	4.1
1	L	213	ASN	4.1
2	M	314	LEU	4.1
2	M	332	VAL	4.1
1	A	124	PHE	4.0
11	K	30	ASN	4.0
5	P	124	HIS	4.0
10	J	42	PRO	4.0
11	V	17	ASP	4.0
11	K	79	GLU	4.0
11	K	76	SER	4.0
11	V	65	SER	3.9
7	G	127	LYS	3.9
1	L	237	VAL	3.9
10	J	31	SER	3.9
11	V	10	SER	3.9
2	B	239	ALA	3.8
1	L	271	ASN	3.8
10	U	75	SER	3.8
11	K	24	ARG	3.8
2	M	213	LYS	3.8
6	F	110	GLN	3.8
11	K	103	LYS	3.8
1	L	124	PHE	3.8
11	V	9	VAL	3.7
4	D	210	PRO	3.7
11	K	83	ILE	3.7
11	V	40	PRO	3.7
8	H	45	VAL	3.7
11	V	100	ALA	3.7
11	V	14	SER	3.7
11	K	40	PRO	3.7
2	B	337	GLU	3.7
9	T	56	ILE	3.6
2	M	337	GLU	3.6
2	M	344	LYS	3.6
2	B	314	LEU	3.6
1	A	398	GLY	3.6
9	T	55	ARG	3.6

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Mol	Chain	Res	Type	RSRZ
11	V	86	TYR	3.6
10	J	127	PRO	3.6
5	P	99	ALA	3.6
6	Q	114	TYR	3.6
11	V	42	GLY	3.6
11	V	15	LEU	3.6
11	K	10	SER	3.6
5	E	154	ILE	3.6
12	W	32	GLY	3.6
6	Q	117	LEU	3.6
11	V	28	ASP	3.5
11	V	41	ASP	3.5
11	K	60	SER	3.5
10	J	125	ARG	3.5
6	F	118	GLU	3.5
1	A	225	SER	3.5
10	U	43	GLY	3.5
12	W	67	LYS	3.5
8	H	68	TYR	3.4
11	V	107	LYS	3.4
6	F	114	TYR	3.4
5	P	48	ASP	3.4
10	J	44	ASN	3.4
8	S	38	GLN	3.4
10	U	65	LYS	3.4
4	D	67	HIS	3.4
1	A	31	GLN	3.3
7	G	17	LYS	3.3
5	E	99	ALA	3.3
11	V	60	SER	3.3
4	D	307	PRO	3.3
11	K	89	GLN	3.3
11	V	3	GLU	3.3
1	L	457	TRP	3.3
1	A	81	GLU	3.3
12	W	34	PRO	3.3
8	H	48	SER	3.3
2	M	211	ALA	3.3
3	C	156	PHE	3.3
12	W	53	LYS	3.3
10	J	1	GLU	3.3
11	K	29	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
3	C	383	VAL	3.2
7	G	20	VAL	3.2
2	B	329	ASN	3.2
6	F	115	ALA	3.2
11	K	35	TRP	3.2
11	K	14	SER	3.2
5	P	100	ALA	3.2
9	I	5	SER	3.2
11	K	106	ILE	3.1
2	M	343	VAL	3.1
11	K	41	ASP	3.1
11	V	4	LEU	3.1
2	M	334	SER	3.1
6	Q	115	ALA	3.1
10	U	127	PRO	3.1
5	E	91	MET	3.1
1	L	111	GLY	3.1
5	E	103	LEU	3.1
10	U	87	THR	3.1
1	L	35	GLY	3.1
2	M	329	ASN	3.0
5	P	45	GLU	3.0
11	V	83	ILE	3.0
9	T	54	ALA	3.0
1	L	236	PRO	3.0
9	I	54	ALA	3.0
3	N	346	VAL	3.0
5	E	97	ASN	3.0
11	K	4	LEU	3.0
10	U	15	SER	3.0
10	U	114	GLN	3.0
2	M	202	ASP	3.0
2	B	339	ASN	3.0
11	V	77	ASN	3.0
1	A	401	LEU	2.9
11	V	70	ASP	2.9
11	K	61	ARG	2.9
11	K	18	ARG	2.9
2	M	238	VAL	2.9
6	F	117	LEU	2.9
6	F	111	GLN	2.9
11	K	100	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
10	J	76	LYS	2.9
5	E	209	GLY	2.9
9	T	5	SER	2.9
2	M	341	ASP	2.9
6	Q	112	PRO	2.9
11	V	74	THR	2.8
12	W	54	GLY	2.8
1	A	217	GLU	2.8
10	J	68	LEU	2.8
6	F	120	LYS	2.8
11	V	89	GLN	2.8
5	P	103	LEU	2.8
8	S	37	LEU	2.8
1	L	240	LYS	2.8
1	A	129	ALA	2.8
2	M	218	LYS	2.8
8	S	56	PHE	2.8
9	T	10	PHE	2.8
4	D	70	HIS	2.8
1	A	76	ILE	2.8
5	P	154	ILE	2.8
11	K	87	PHE	2.8
12	W	12	ALA	2.8
2	B	218	LYS	2.8
12	W	17	THR	2.7
10	U	76	LYS	2.7
7	G	90	ARG	2.7
1	L	122	GLN	2.7
3	N	307	PHE	2.7
2	B	215	LEU	2.7
1	A	210	GLY	2.7
10	J	57	ASP	2.7
2	M	239	ALA	2.7
10	U	44	ASN	2.7
10	J	30	THR	2.7
2	B	312	LYS	2.7
5	E	40	ASP	2.6
2	B	241	ILE	2.6
10	U	88	THR	2.6
12	W	9	PRO	2.6
12	W	13	LYS	2.6
12	W	98	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
3	C	346	VAL	2.6
4	D	207	ALA	2.6
1	L	44	PRO	2.6
2	B	238	VAL	2.6
10	U	45	LYS	2.6
5	E	124	HIS	2.6
11	K	26	SER	2.6
8	S	6	GLY	2.6
8	S	84	ALA	2.6
9	I	6	LEU	2.6
1	L	235	LYS	2.5
11	K	70	ASP	2.5
2	B	51	LEU	2.5
10	U	125	ARG	2.5
4	D	211	GLY	2.5
11	K	23	CYS	2.5
1	A	44	PRO	2.5
5	E	208	ASP	2.5
5	P	105	LYS	2.5
8	H	37	LEU	2.5
5	E	188	SER	2.5
1	A	213	ASN	2.5
5	P	97	ASN	2.5
1	L	135	SER	2.5
10	U	35	TRP	2.5
1	A	232	THR	2.5
1	A	226	LYS	2.5
11	K	39	LYS	2.5
9	T	9	THR	2.5
4	D	138	PRO	2.4
11	V	81	GLU	2.4
5	E	48	ASP	2.4
10	U	37	TRP	2.4
9	I	12	LYS	2.4
1	A	215	LYS	2.4
1	L	241	LYS	2.4
10	U	62	PRO	2.4
11	K	64	GLY	2.4
2	B	219	SER	2.4
2	B	25	PRO	2.4
7	R	17	LYS	2.4
1	L	227	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
7	R	24	LEU	2.4
10	J	18	LEU	2.4
10	J	9	ALA	2.4
2	B	335	PRO	2.3
5	E	102	PRO	2.3
5	P	102	PRO	2.3
2	B	166	ARG	2.3
11	V	23	CYS	2.3
12	W	73	MET	2.3
11	K	80	PRO	2.3
12	W	30	GLU	2.3
10	J	49	VAL	2.3
2	M	61	THR	2.3
12	W	14	LYS	2.3
12	W	82	LYS	2.3
1	A	224	GLU	2.3
1	L	150	ASP	2.3
2	B	293	ASP	2.3
5	P	208	ASP	2.3
6	Q	103	GLU	2.3
10	U	57	ASP	2.3
11	K	21	ILE	2.3
11	V	82	ASP	2.3
1	A	405	GLU	2.3
2	M	240	ALA	2.3
2	M	335	PRO	2.3
8	H	7	LYS	2.3
3	N	156	PHE	2.3
11	K	81	GLU	2.3
6	Q	74	VAL	2.3
11	K	7	THR	2.3
11	K	85	THR	2.3
11	V	35	TRP	2.3
8	S	5	SER	2.3
1	L	88	LYS	2.3
2	B	321	THR	2.3
2	M	195	ALA	2.2
5	P	213	ILE	2.2
1	A	271	ASN	2.2
11	K	90	HIS	2.2
11	K	28	ASP	2.2
8	S	51	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
4	O	307	PRO	2.2
8	H	84	ALA	2.2
6	Q	110	GLN	2.2
1	L	34	ASN	2.2
10	J	43	GLY	2.2
2	M	166	ARG	2.2
4	D	140	GLU	2.2
1	L	397	LYS	2.2
11	K	77	ASN	2.2
5	E	45	GLU	2.2
11	V	66	GLY	2.2
1	L	238	LEU	2.2
11	K	36	TYR	2.2
11	V	84	ALA	2.2
6	Q	116	ASP	2.2
2	B	334	SER	2.2
7	R	10	ARG	2.2
11	K	92	ILE	2.2
6	Q	111	GLN	2.2
8	H	51	ARG	2.2
12	W	97	GLU	2.2
11	K	74	THR	2.2
11	V	61	ARG	2.2
6	F	74	VAL	2.2
2	M	241	ILE	2.2
1	A	408	LYS	2.2
10	J	3	LYS	2.2
11	V	43	THR	2.2
4	D	209	PRO	2.2
7	R	20	VAL	2.1
2	B	292	GLN	2.1
2	B	136	GLN	2.1
2	B	154	GLY	2.1
12	W	10	GLY	2.1
4	D	62	MET	2.1
5	E	213	ILE	2.1
2	M	220	GLU	2.1
2	M	339	ASN	2.1
10	J	74	THR	2.1
11	K	88	CYS	2.1
5	E	118	ILE	2.1
7	R	118	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
11	K	1	ASP	2.1
12	W	59	ASP	2.1
1	A	397	LYS	2.1
2	M	321	THR	2.1
11	V	57	GLY	2.1
1	L	33	SER	2.1
2	M	22	ARG	2.1
1	A	72	LEU	2.1
9	I	10	PHE	2.1
1	L	232	THR	2.1
1	L	221	ASN	2.1
1	A	236	PRO	2.1
11	K	43	THR	2.1
5	E	211	LYS	2.1
1	A	237	VAL	2.1
1	L	130	ASN	2.1
4	O	70	HIS	2.1
3	C	307	PHE	2.1
11	V	33	LEU	2.1
6	F	108	GLN	2.0
10	U	13	GLN	2.0
2	B	187	VAL	2.0
4	O	306	LYS	2.0
2	B	266	GLU	2.0
12	W	111	ALA	2.0
1	L	424	LYS	2.0
11	V	75	ILE	2.0
1	A	351	TRP	2.0
1	A	33	SER	2.0
2	B	344	LYS	2.0
2	M	312	LYS	2.0
1	A	35	GLY	2.0
4	O	137	GLU	2.0
4	O	141	GLN	2.0
11	V	78	LEU	2.0
1	L	215	LYS	2.0
11	K	32	PHE	2.0
11	K	93	LYS	2.0
11	V	71	TYR	2.0
1	A	227	ASN	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
12	M3L	W	81	12/13	0.89	0.30	-	60,63,64,66	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
19	9PE	N	4011	40/40	0.94	0.19	2.61	50,54,63,64	0
13	SUC	O	4146	23/23	0.80	0.30	2.47	72,77,80,81	0
19	9PE	C	4111	40/40	0.92	0.17	2.28	45,57,75,76	0
20	7PH	D	4014	38/38	0.93	0.21	1.54	48,53,61,62	0
20	7PH	O	4114	38/38	0.93	0.20	1.52	38,44,51,54	0
18	CN6	C	4031	50/50	0.87	0.23	1.46	50,70,78,80	0
22	6PH	L	4113	40/40	0.90	0.17	1.24	49,60,69,69	0
17	8PE	N	4110	47/47	0.91	0.19	0.95	28,65,74,75	0
22	6PH	E	4013	40/40	0.89	0.17	0.55	56,65,72,72	0
17	8PE	C	4010	47/47	0.91	0.17	0.45	39,59,62,65	0
18	CN6	N	4131	50/50	0.89	0.21	0.26	53,67,77,79	0
16	SMA	C	4005	37/37	0.96	0.14	0.02	29,33,37,37	0
14	UMQ	L	4121	34/34	0.94	0.15	-0.08	39,44,59,60	0
14	UMQ	A	4021	34/34	0.94	0.16	-0.19	42,48,65,67	0
16	SMA	N	4025	37/37	0.97	0.13	-0.23	23,28,31,32	0
15	HEM	D	4003	43/43	0.98	0.13	-0.37	35,39,43,44	0
15	HEM	W	4026	43/43	0.96	0.16	-0.44	47,55,57,58	0
15	HEM	C	4001	43/43	0.99	0.12	-0.61	21,26,32,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
15	HEM	O	4023	43/43	0.99	0.10	-0.81	32,37,41,42	0
15	HEM	N	4022	43/43	0.99	0.11	-0.86	21,23,32,35	0
15	HEM	N	4021	43/43	0.99	0.11	-0.98	15,23,30,34	0
21	FES	E	4004	4/4	0.99	0.13	-1.01	30,32,32,37	0
15	HEM	C	4002	43/43	0.99	0.11	-1.13	20,26,37,37	0
21	FES	P	4024	4/4	0.99	0.10	-1.63	32,36,36,37	0

6.5 Other polymers

There are no such residues in this entry.