Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:04 AM GMT

PDB ID	:	3CX5
Title	:	Structure of complex III with bound cytochrome c in reduced state and definition of a minimal core interface for electron transfer.
Authors	:	Solmaz, S.R.N.; Hunte, C.
Deposited on	:	2008-04-23
Resolution	:	1.90 Å(reported)

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

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

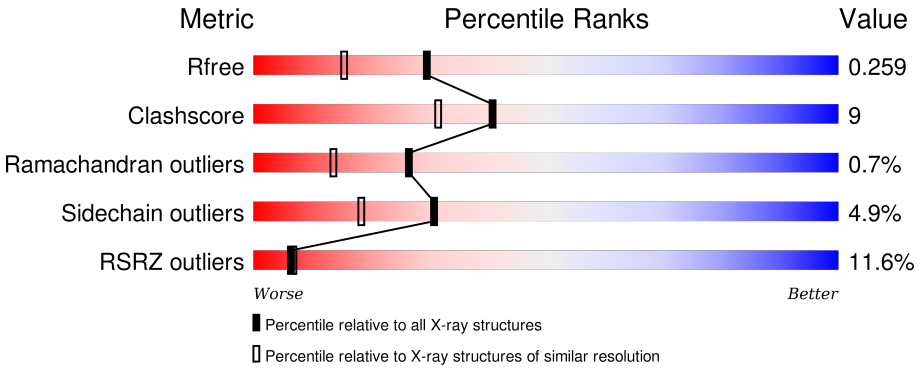
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.90 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	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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	12% 79% 19%
1	L	431	10% 76% 20%
2	B	352	10% 76% 22%
2	M	352	10% 72% 25%
3	C	385	% 84% 15%

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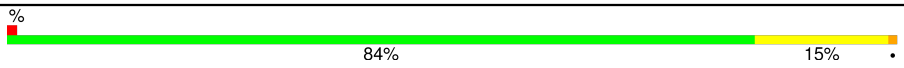
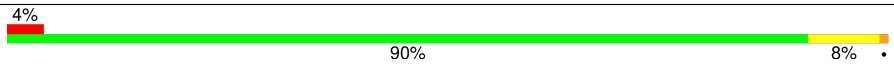
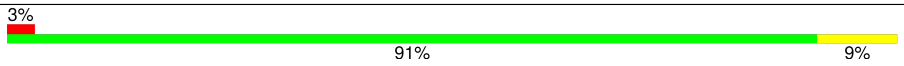
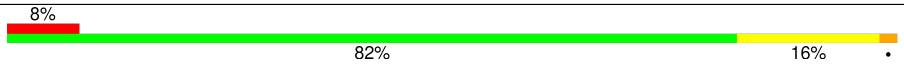
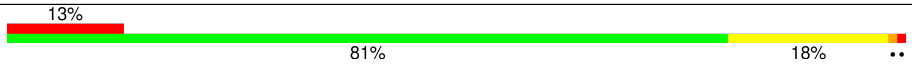
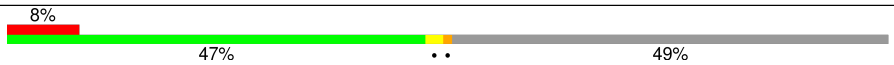
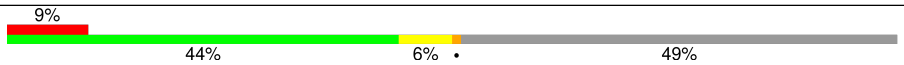
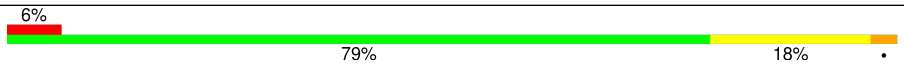
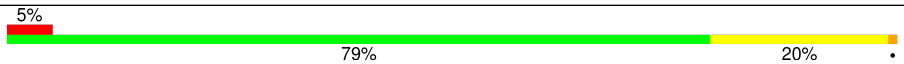
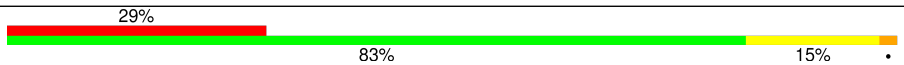
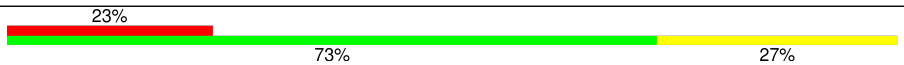
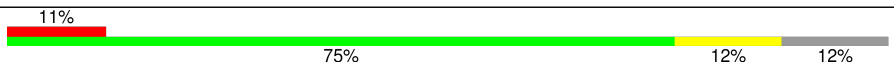
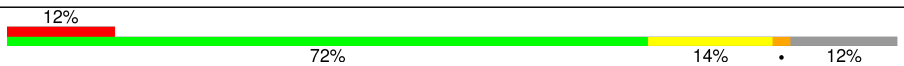
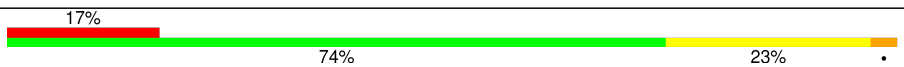
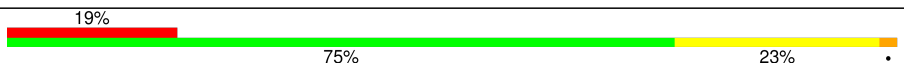
Mol	Chain	Length	Quality of chain
3	N	385	
4	D	248	
4	O	248	
5	E	185	
5	P	185	
6	F	146	
6	Q	146	
7	G	126	
7	R	126	
8	H	93	
8	S	93	
9	I	65	
9	T	65	
10	J	127	
10	U	127	
11	K	107	
11	V	107	
12	W	108	

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
18	8PE	N	4110	-	-	-	X
19	9PE	N	4111	-	-	-	X
20	CN5	C	4033	-	-	-	X
21	7PH	D	4014	-	-	-	X
21	7PH	O	4114	-	-	-	X

2 Entry composition

There are 24 unique types of molecules in this entry. The entry contains 38020 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	248	Total	C	N	O	S	0	0	0
			1961	1249	340	363	9			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	O	248	Total	C	N	O	S	0	0	0
			1961	1249	340	363	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	126	Total	C	N	O	S	0	0	0
			1019	653	173	191	2			
7	R	126	Total	C	N	O	S	0	0	0
			1019	653	173	191	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	57	Total	C	N	O	0	0	0
			465	310	77	78			
9	T	57	Total	C	N	O	0	0	0
			465	310	77	78			

- 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			

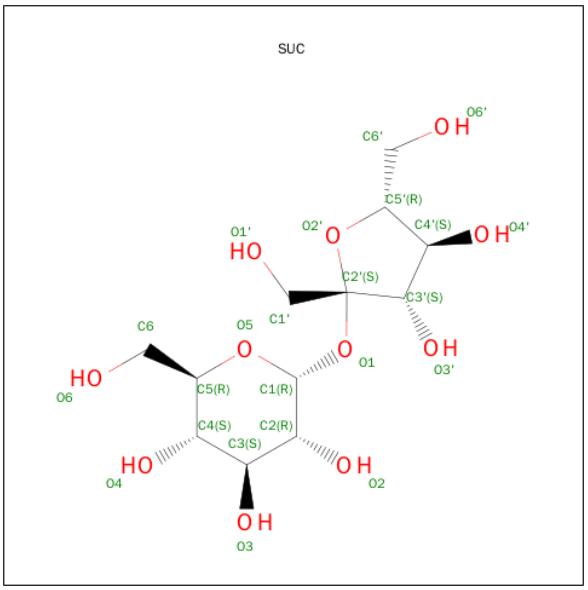
- Molecule 11 is a protein called LIGHT CHAIN (VL) OF FV-FRAGMENT.

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-1.

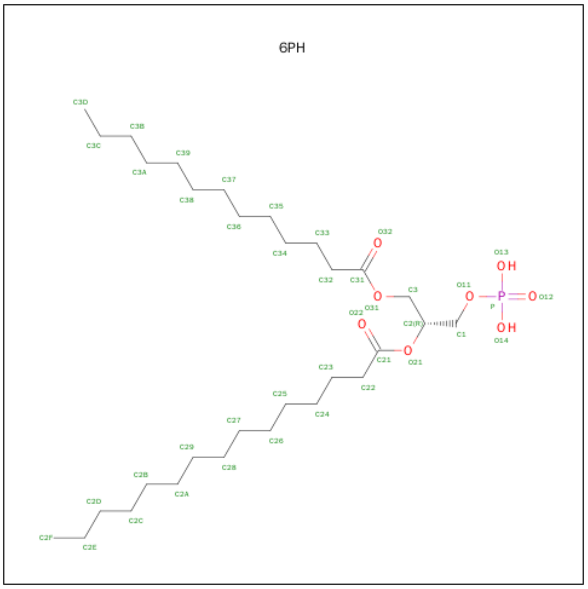
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	W	108	Total	C	N	O	S	0	1	0
			859	542	153	159	5			

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



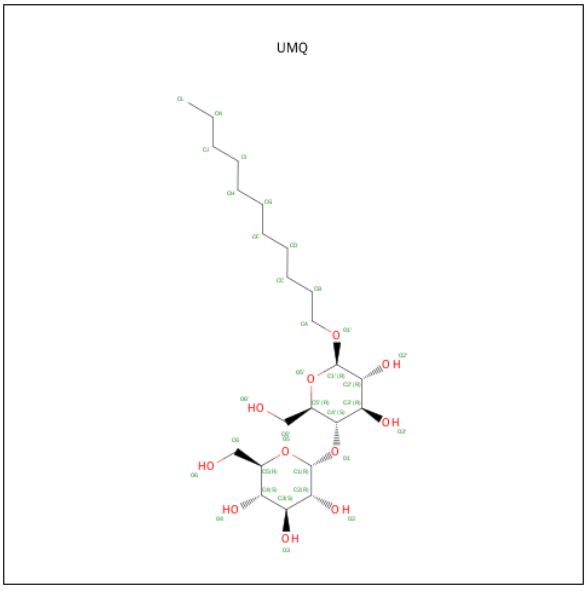
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	O	1	Total	C	O	0	0
			23	12	11		

- Molecule 14 is (1R)-2-(PHOSPHONOOXY)-1-[(TRIDECANOYLOXY)METHYL]ETHYL PENTADECANOATE (three-letter code: 6PH) (formula: $C_{31}H_{61}O_8P$).



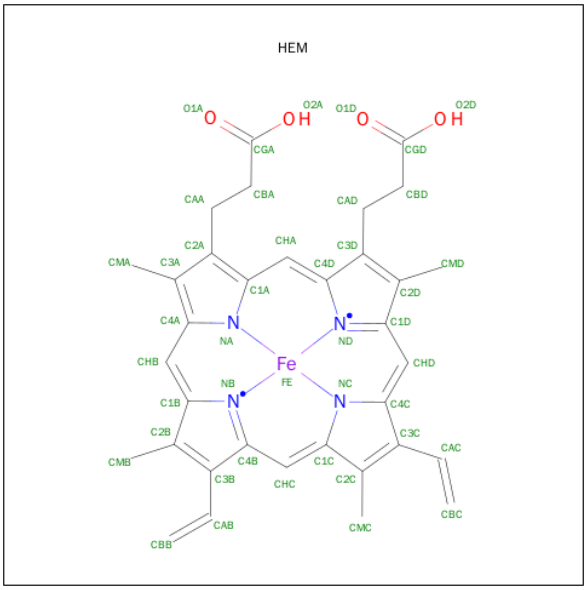
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	A	1	Total	C	O	P	0	0
			40	31	8	1		
14	L	1	Total	C	O	P	0	0
			40	31	8	1		

- Molecule 15 is UNDECYL-MALTOSIDE (three-letter code: UMQ) (formula: $C_{23}H_{44}O_{11}$).



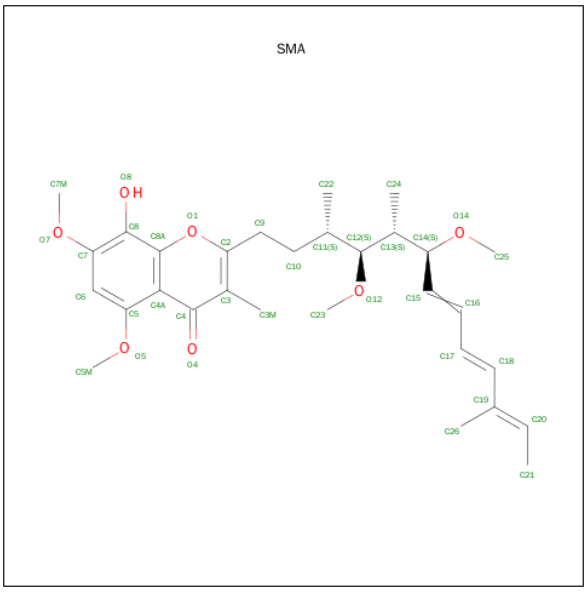
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	A	1	Total C O 34 23 11	0	0
15	L	1	Total C O 34 23 11	0	0

- Molecule 16 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



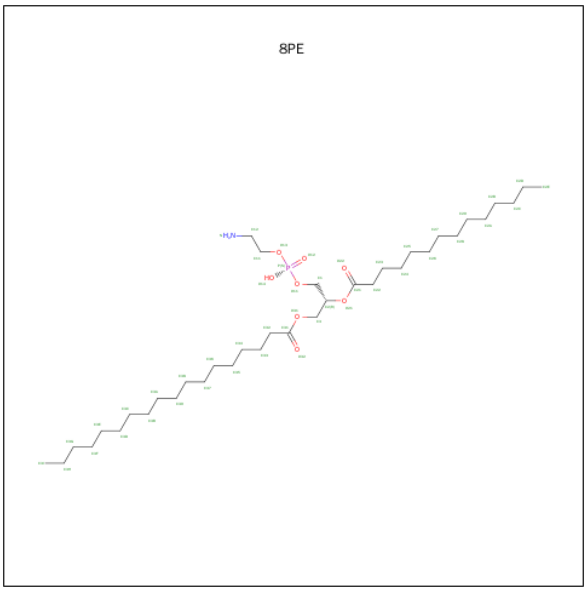
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	C	1	Total C Fe N O 43 34 1 4 4	0	0
16	C	1	Total C Fe N O 43 34 1 4 4	0	0
16	D	1	Total C Fe N O 43 34 1 4 4	0	0
16	N	1	Total C Fe N O 43 34 1 4 4	0	0
16	N	1	Total C Fe N O 43 34 1 4 4	0	0
16	O	1	Total C Fe N O 43 34 1 4 4	0	0
16	W	1	Total C Fe N O 43 34 1 4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

- Molecule 17 is STIGMATELLIN A (three-letter code: SMA) (formula: $C_{30}H_{42}O_7$).



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

- Molecule 18 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
18	C	1	Total C N O P 47 37 1 8 1	0	0

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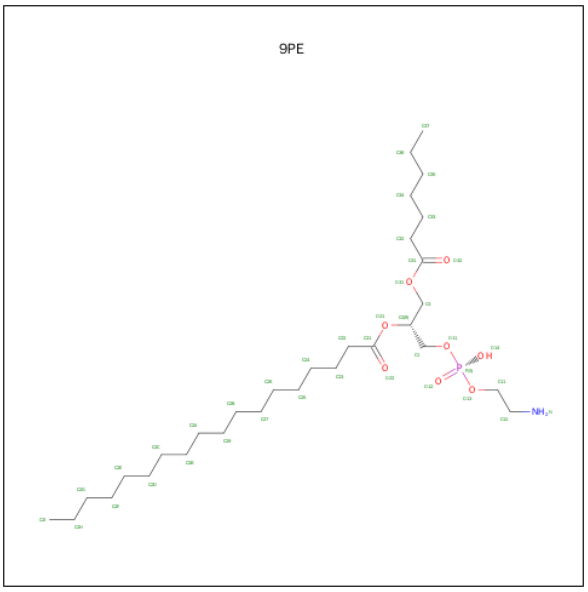
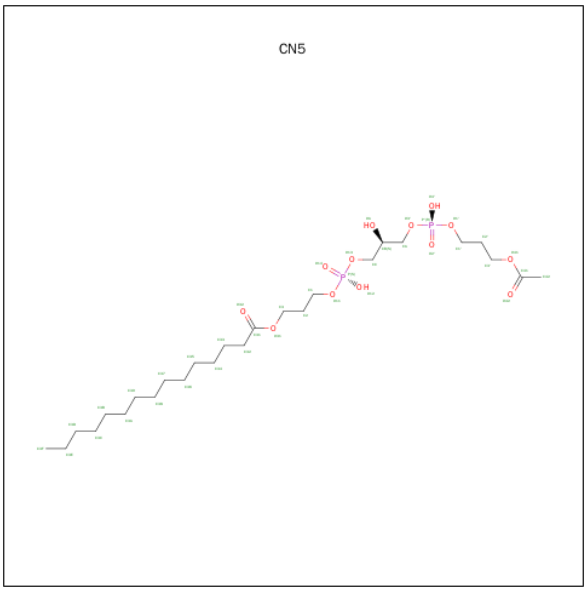
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	N	1	Total	C	N	O	P	0	0
			47	37	1	8	1		

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



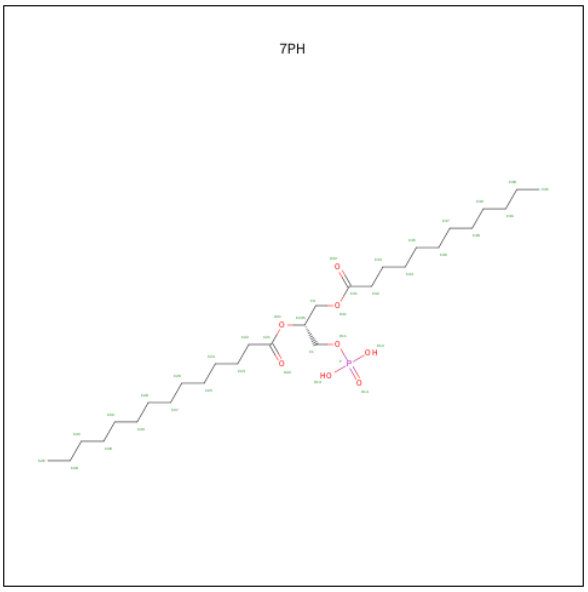
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	C	1	Total	C	N	O	P	0	0
			40	30	1	8	1		
19	N	1	Total	C	N	O	P	0	0
			40	30	1	8	1		

- Molecule 20 is (5S,11R)-5,8,11-TRIHYDROXY-5,11-DIOXIDO-17-OXO-4,6,10,12,16-PENTAOXA-5,11-DIPHOSPHAOCTADEC-1-YL PENTADECANOATE (three-letter code: CN5) (formula: $C_{26}H_{52}O_{13}P_2$).



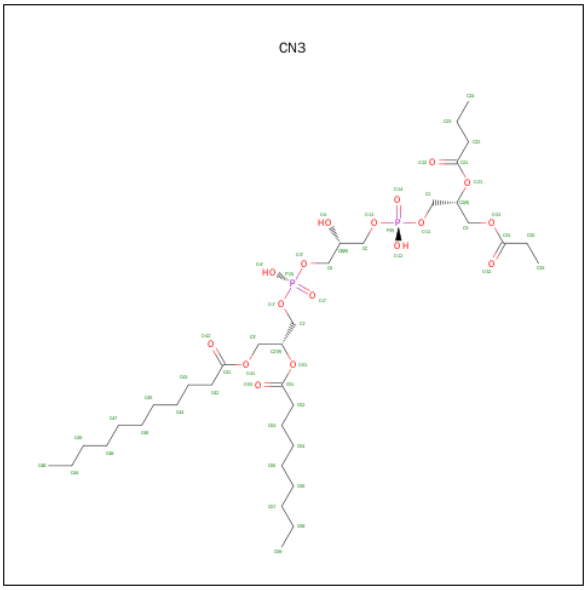
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	C	1	Total	C	O	P	0	0
			41	26	13	2		

- Molecule 21 is (1R)-2-(DODECANOYLOXY)-1-[(PHOSPHONOOXY)METHYL]ETHYL TETRADECANOATE (three-letter code: 7PH) (formula: $C_{29}H_{57}O_8P$).



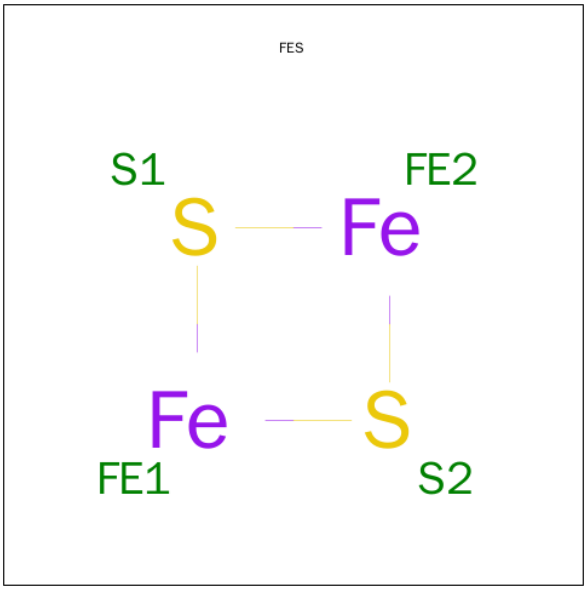
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
21	D	1	Total	C	O	P	0	0
			38	29	8	1		
21	O	1	Total	C	O	P	0	0
			38	29	8	1		

- Molecule 22 is (2R,5S,11R,14R)-5,8,11-TRIHYDROXY-2-(NONANOYLOXY)-5,11-DIOXIDO-16-OXO-14-[(PROPANOYLOXY)METHYL]-4,6,10,12,15-PENTAOXA-5,11-DIPHOSPHANONADEC-1-YL UNDECANOATE (three-letter code: CN3) (formula: $C_{36}H_{68}O_{17}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
22	D	1	Total	C	O	P	0	0
			55	36	17	2		
22	N	1	Total	C	O	P	0	0
			55	36	17	2		

- Molecule 23 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



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

- Molecule 24 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	153	Total O 153 153	0	0
24	B	93	Total O 93 93	0	0
24	C	161	Total O 161 161	0	0
24	D	154	Total O 154 154	0	0
24	E	74	Total O 74 74	0	0
24	F	16	Total O 16 16	0	0
24	G	71	Total O 71 71	0	0
24	H	31	Total O 31 31	0	0
24	I	11	Total O 11 11	0	0
24	J	15	Total O 15 15	0	0
24	K	7	Total O 7 7	0	0
24	L	170	Total O 170 170	0	0
24	M	101	Total O 101 101	0	0
24	N	170	Total O 170 170	0	0
24	O	173	Total O 173 173	0	0
24	P	66	Total O 66 66	0	0
24	Q	27	Total O 27 27	0	0
24	R	73	Total O 73 73	0	0

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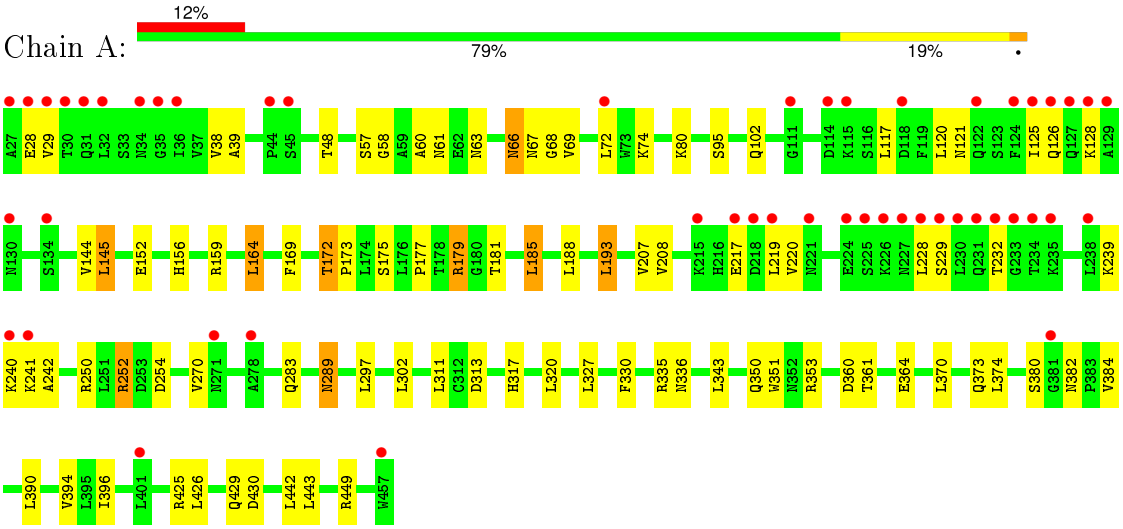
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	S	40	Total O 40 40	0	0
24	T	12	Total O 12 12	0	0
24	U	8	Total O 8 8	0	0
24	V	2	Total O 2 2	0	0
24	W	20	Total O 20 20	0	0

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.

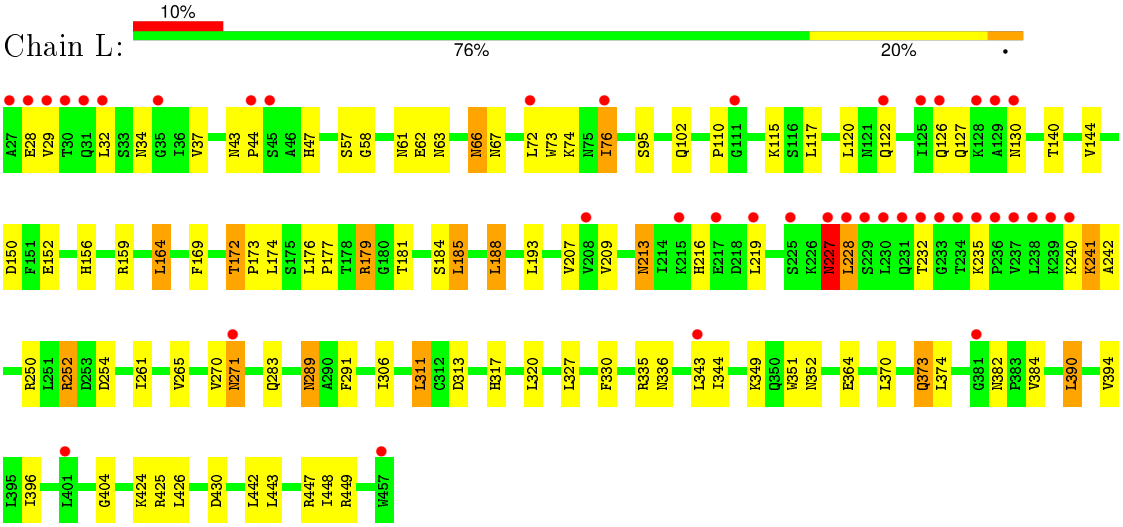
- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain A:



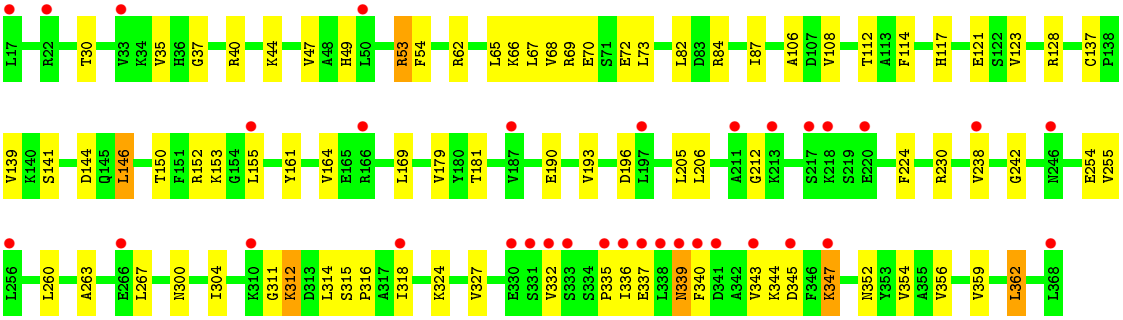
- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain L:

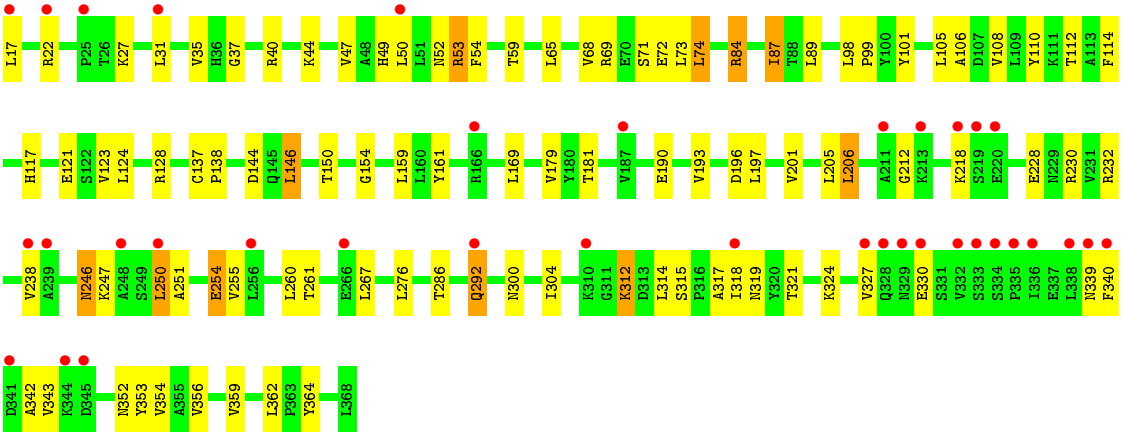


- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

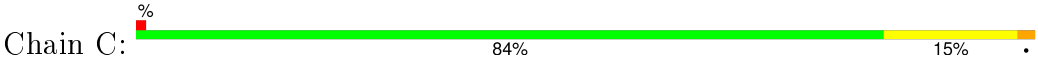
Chain B:

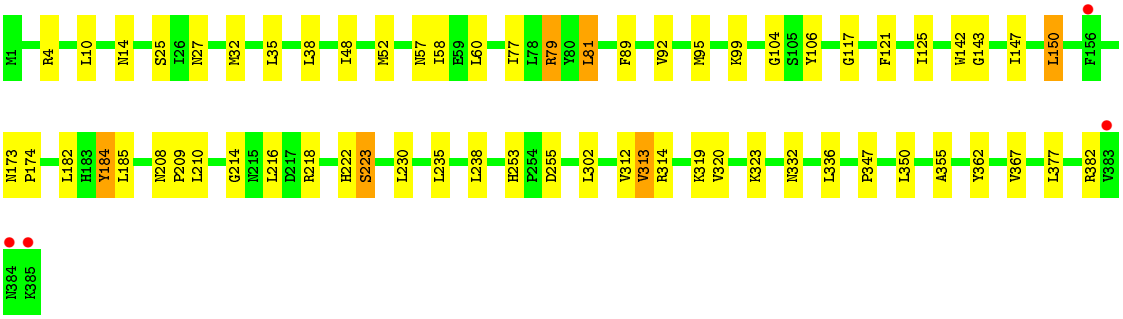


• Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

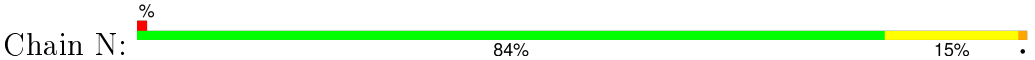


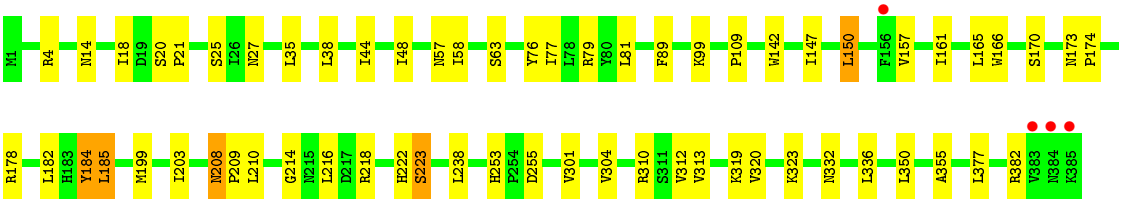
• Molecule 3: CYTOCHROME B





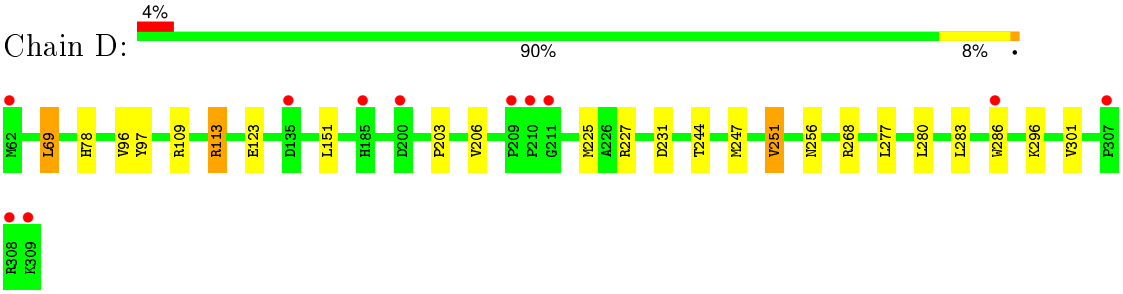
• Molecule 3: CYTOCHROME B





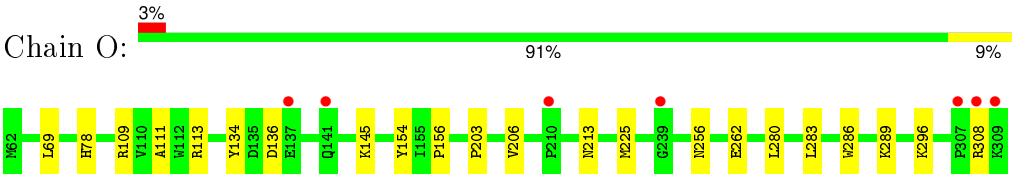
• Molecule 4: Cytochrome c1, heme protein, mitochondrial

Chain D:



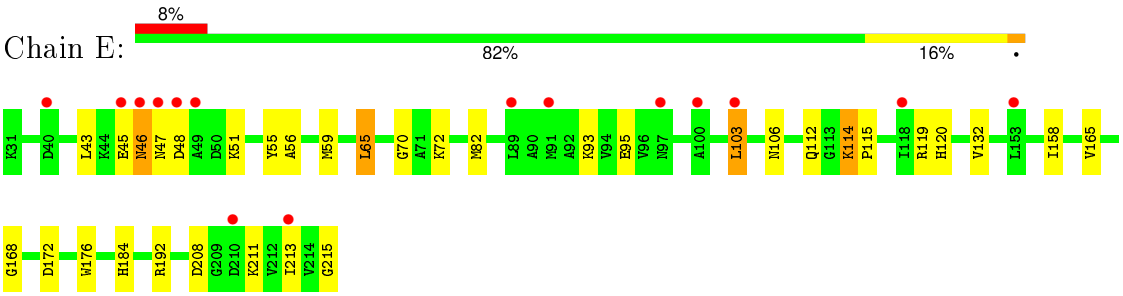
• Molecule 4: Cytochrome c1, heme protein, mitochondrial

Chain O:



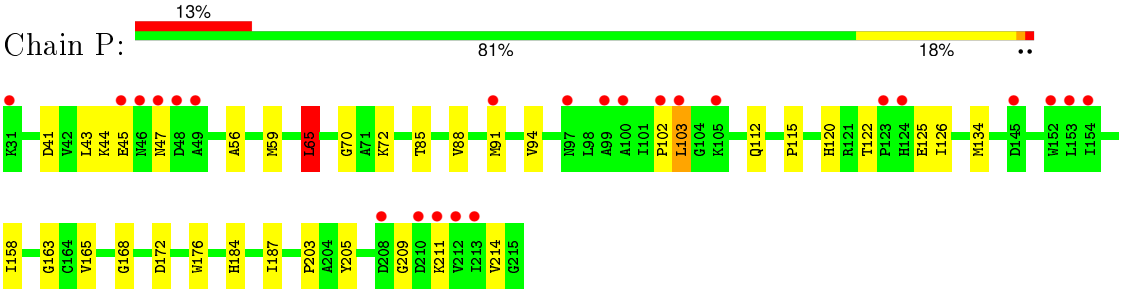
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain E:



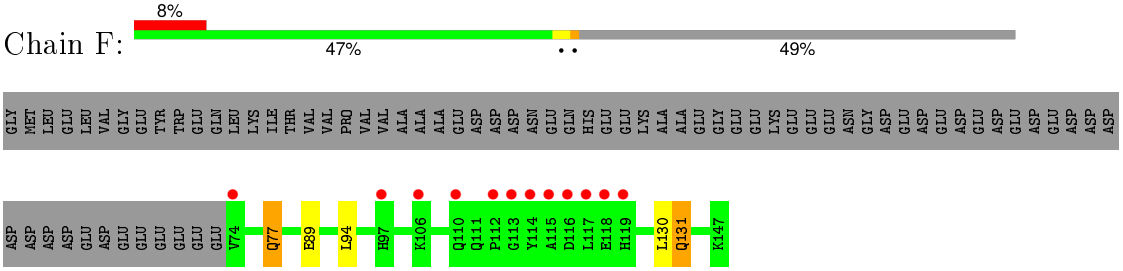
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain P:



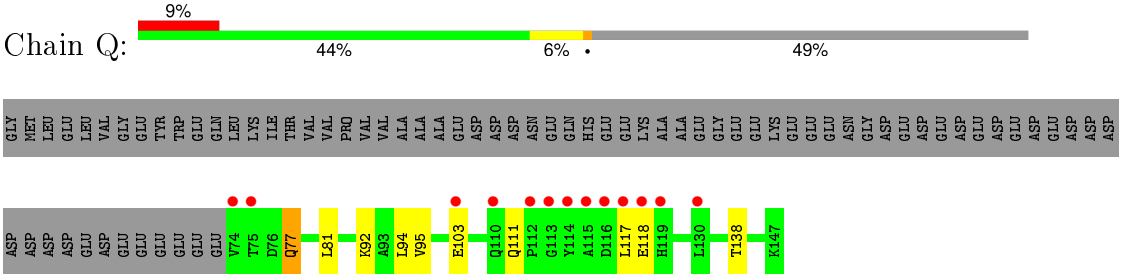
• Molecule 6: Cytochrome b-c1 complex subunit 6

Chain F:



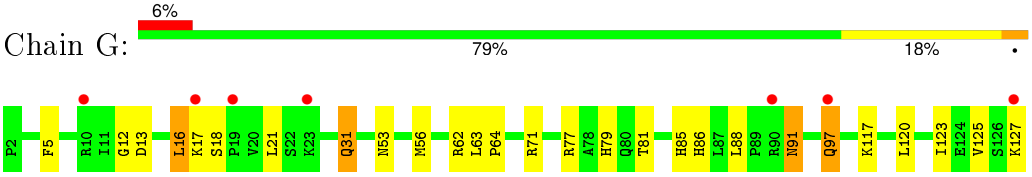
• Molecule 6: Cytochrome b-c1 complex subunit 6

Chain Q:



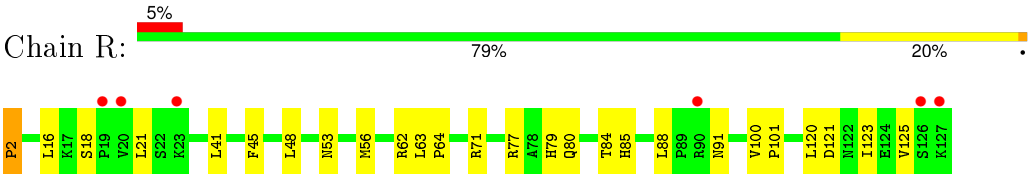
• Molecule 7: Cytochrome b-c1 complex subunit 7

Chain G:



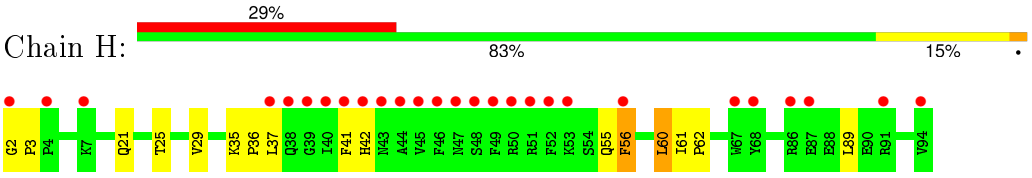
• Molecule 7: Cytochrome b-c1 complex subunit 7

Chain R:



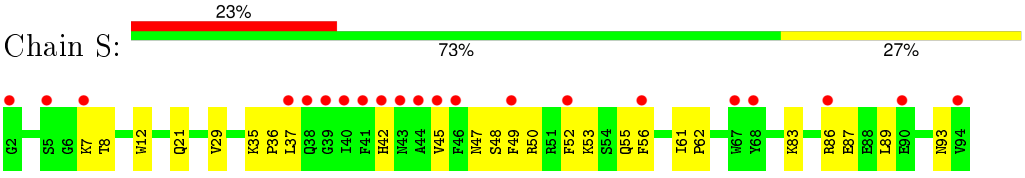
• Molecule 8: Cytochrome b-c1 complex subunit 8

Chain H:



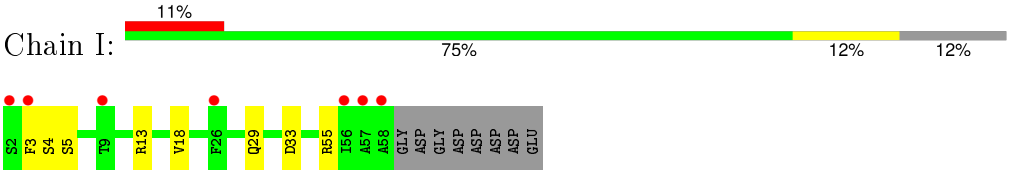
• Molecule 8: Cytochrome b-c1 complex subunit 8

Chain S:



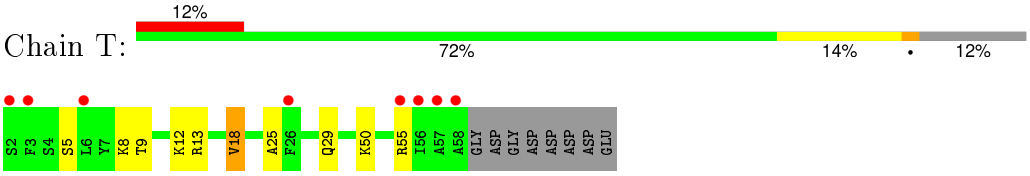
• Molecule 9: Cytochrome b-c1 complex subunit 9

Chain I:



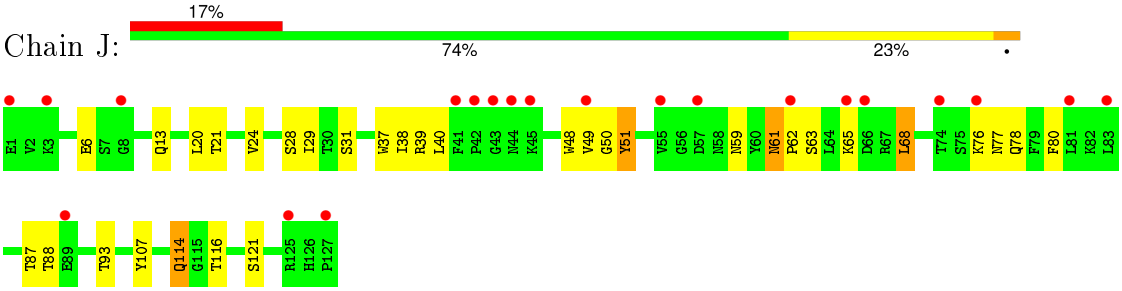
• Molecule 9: Cytochrome b-c1 complex subunit 9

Chain T:



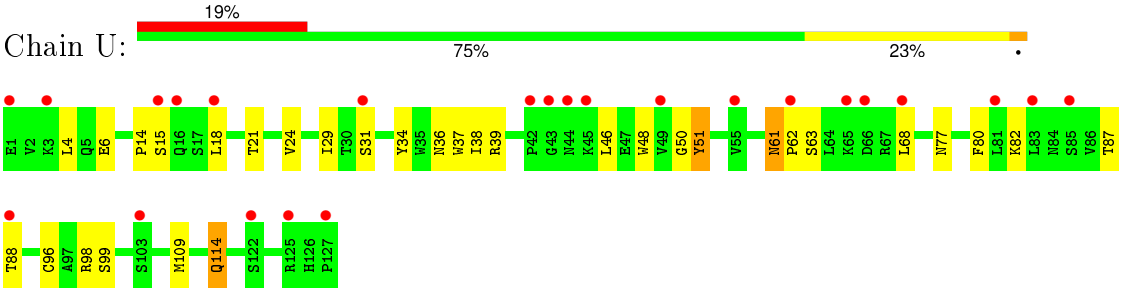
• Molecule 10: HEAVY CHAIN (VH) OF FV-FRAGMENT

Chain J:



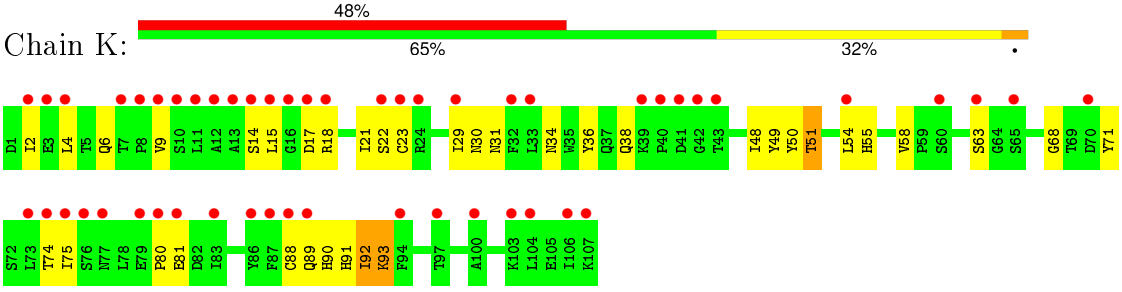
• Molecule 10: HEAVY CHAIN (VH) OF FV-FRAGMENT

Chain U:



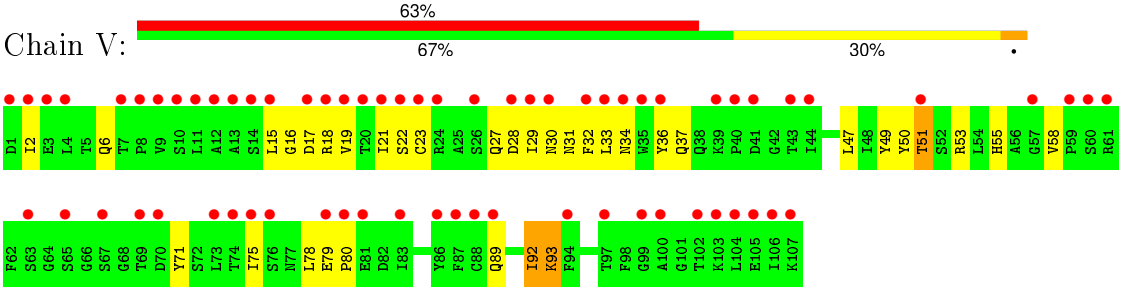
• Molecule 11: LIGHT CHAIN (VL) OF FV-FRAGMENT

Chain K:



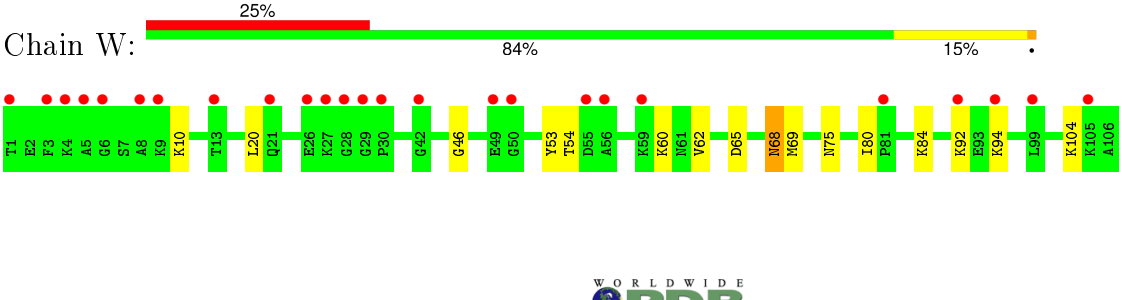
• Molecule 11: LIGHT CHAIN (VL) OF FV-FRAGMENT

Chain V:



• Molecule 12: Cytochrome c iso-1

Chain W:




C107
E108

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	145.12Å 165.09Å 194.37Å 90.00° 104.09° 90.00°	Depositor
Resolution (Å)	18.99 – 1.90 18.99 – 1.90	Depositor EDS
% Data completeness (in resolution range)	95.0 (18.99-1.90) 95.2 (18.99-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	1.33 (at 1.90Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.245 , 0.263 0.242 , 0.259	Depositor DCC
R_{free} test set	33007 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	30.5	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 56.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	7 of 660107 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	38020	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.34% 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: CN5, UMQ, CN3, 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	0.34	0/3405	0.60	0/4614
1	L	0.35	0/3405	0.60	1/4614 (0.0%)
2	B	0.33	0/2781	0.60	1/3764 (0.0%)
2	M	0.34	0/2781	0.61	1/3764 (0.0%)
3	C	0.42	0/3192	0.63	1/4354 (0.0%)
3	N	0.43	0/3192	0.62	0/4354
4	D	0.36	0/2022	0.60	0/2751
4	O	0.37	0/2022	0.61	0/2751
5	E	0.34	0/1444	0.58	1/1957 (0.1%)
5	P	0.34	0/1444	0.58	2/1957 (0.1%)
6	F	0.33	0/638	0.49	0/858
6	Q	0.34	0/638	0.49	0/858
7	G	0.33	0/1040	0.60	1/1408 (0.1%)
7	R	0.36	0/1040	0.61	1/1408 (0.1%)
8	H	0.38	0/804	0.51	0/1088
8	S	0.37	0/804	0.53	0/1088
9	I	0.39	0/479	0.46	0/646
9	T	0.41	0/479	0.50	0/646
10	J	0.33	0/1043	0.60	0/1422
10	U	0.33	0/1043	0.59	0/1422
11	K	0.31	0/863	0.50	0/1172
11	V	0.30	0/863	0.51	0/1172
12	W	0.31	0/865	0.54	0/1157
All	All	0.36	0/36287	0.59	9/49225 (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
4	D	0	1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	314	ARG	NE-CZ-NH1	-6.89	116.85	120.30
2	M	87	ILE	N-CA-C	-6.26	94.09	111.00
2	B	87	ILE	N-CA-C	-5.98	94.86	111.00
5	E	65	LEU	CA-CB-CG	5.74	128.49	115.30
7	R	71	ARG	NE-CZ-NH1	-5.70	117.45	120.30
5	P	65	LEU	CA-CB-CG	5.60	128.18	115.30
5	P	163	GLY	N-CA-C	5.26	126.26	113.10
7	G	71	ARG	NE-CZ-NH1	-5.20	117.70	120.30
1	L	447	ARG	NE-CZ-NH1	-5.12	117.74	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	97	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	62	0
1	L	3344	0	3321	76	0
2	B	2735	0	2774	69	0
2	M	2735	0	2774	70	0
3	C	3090	0	3129	43	0
3	N	3090	0	3129	40	0
4	D	1961	0	1888	21	0
4	O	1961	0	1888	16	0
5	E	1411	0	1386	28	0
5	P	1411	0	1386	27	0
6	F	624	0	581	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	Q	624	0	581	6	0
7	G	1019	0	1034	22	0
7	R	1019	0	1034	19	0
8	H	773	0	736	10	0
8	S	773	0	736	18	0
9	I	465	0	459	7	0
9	T	465	0	459	9	0
10	J	1015	0	959	29	0
10	U	1015	0	959	25	0
11	K	842	0	820	28	0
11	V	842	0	820	25	0
12	W	859	0	862	13	0
13	O	23	0	22	5	0
14	A	40	0	59	1	0
14	L	40	0	59	3	0
15	A	34	0	44	2	0
15	L	34	0	44	2	0
16	C	86	0	60	2	0
16	D	43	0	30	1	0
16	N	86	0	60	3	0
16	O	43	0	30	0	0
16	W	43	0	30	0	0
17	C	37	0	42	1	0
17	N	37	0	42	0	0
18	C	47	0	73	1	0
18	N	47	0	73	0	0
19	C	40	0	59	0	0
19	N	40	0	59	0	0
20	C	41	0	50	5	0
21	D	38	0	55	2	0
21	O	38	0	55	2	0
22	D	55	0	66	5	0
22	N	55	0	66	5	0
23	E	4	0	0	0	0
23	P	4	0	0	0	0
24	A	153	0	0	2	0
24	B	93	0	0	8	0
24	C	161	0	0	2	0
24	D	154	0	0	5	0
24	E	74	0	0	0	0
24	F	16	0	0	0	0
24	G	71	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	H	31	0	0	0	0
24	I	11	0	0	0	0
24	J	15	0	0	0	0
24	K	7	0	0	0	0
24	L	170	0	0	0	0
24	M	101	0	0	1	0
24	N	170	0	0	1	0
24	O	173	0	0	6	0
24	P	66	0	0	2	0
24	Q	27	0	0	0	0
24	R	73	0	0	1	0
24	S	40	0	0	0	0
24	T	12	0	0	1	0
24	U	8	0	0	0	0
24	V	2	0	0	0	0
24	W	20	0	0	0	0
All	All	38020	0	36114	620	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 9.

All (620) 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:B:150:THR:HG22	2:B:352:ASN:HD22	1.27	1.00
2:M:246:ASN:HD22	2:M:246:ASN:H	1.11	0.99
2:M:150:THR:HG22	2:M:352:ASN:HD22	1.27	0.97
6:F:77:GLN:H	6:F:77:GLN:HE21	1.12	0.97
2:M:255:VAL:HG12	2:M:321:THR:HG21	1.47	0.96
1:L:63:ASN:H	1:L:66:ASN:HD21	1.10	0.92
1:A:63:ASN:H	1:A:66:ASN:HD21	1.18	0.91
10:J:114:GLN:H	10:J:114:GLN:HE21	1.21	0.88
7:R:77:ARG:HD3	7:R:88:LEU:HD11	1.56	0.88
10:J:29:ILE:H	10:J:77:ASN:HD21	1.16	0.87
6:Q:77:GLN:H	6:Q:77:GLN:HE21	1.14	0.86
13:O:4146:SUC:H1'2	12:W:20:LEU:HD23	1.58	0.86
2:B:318:ILE:HD11	2:B:340:PHE:HB3	1.59	0.84
7:G:77:ARG:HD3	7:G:88:LEU:HD11	1.60	0.84
11:K:31:ASN:HD22	11:K:51:THR:HG21	1.42	0.83
22:N:4131:CN3:HAA	7:R:85:HIS:NE2	1.93	0.83
2:B:150:THR:HG22	2:B:352:ASN:ND2	1.92	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:150:THR:HG22	2:M:352:ASN:ND2	1.92	0.83
12:W:60:LYS:HG3	12:W:62:VAL:HG23	1.62	0.82
1:A:361:THR:HG21	7:R:123:ILE:O	1.80	0.82
1:A:63:ASN:H	1:A:66:ASN:ND2	1.78	0.82
2:B:49:HIS:HD2	2:B:161:TYR:H	1.28	0.81
1:L:317:HIS:HE1	1:L:351:TRP:HE1	1.28	0.80
1:A:179:ARG:HG2	1:A:179:ARG:HH21	1.47	0.80
2:M:246:ASN:H	2:M:246:ASN:ND2	1.80	0.79
2:M:318:ILE:HD11	2:M:340:PHE:HB3	1.65	0.79
6:Q:77:GLN:H	6:Q:77:GLN:NE2	1.81	0.78
1:A:317:HIS:HE1	1:A:351:TRP:HE1	1.30	0.77
2:M:49:HIS:HD2	2:M:161:TYR:H	1.33	0.77
3:N:58:ILE:H	3:N:173:ASN:HD22	1.29	0.77
10:U:29:ILE:H	10:U:77:ASN:HD21	1.32	0.77
1:L:63:ASN:H	1:L:66:ASN:ND2	1.82	0.77
7:G:31:GLN:HA	7:G:31:GLN:HE21	1.50	0.77
6:F:77:GLN:H	6:F:77:GLN:NE2	1.82	0.76
4:O:225:MET:HE2	24:O:5654:HOH:O	1.85	0.76
1:A:58:GLY:H	1:A:61:ASN:HD22	1.32	0.76
22:D:4031:CN3:HAA	7:G:85:HIS:NE2	2.02	0.75
3:N:214:GLY:O	3:N:218:ARG:HD2	1.87	0.75
2:B:37:GLY:HA3	2:B:179:VAL:HG11	1.69	0.75
2:B:108:VAL:O	2:B:112:THR:HG23	1.86	0.75
2:B:238:VAL:HG13	2:B:356:VAL:HB	1.68	0.74
2:M:37:GLY:HA3	2:M:179:VAL:HG11	1.68	0.74
10:J:6:GLU:H	10:J:114:GLN:HE22	1.35	0.74
5:P:172:ASP:H	5:P:184:HIS:HD2	1.36	0.74
4:D:96:VAL:HB	4:D:251:VAL:HG13	1.70	0.73
5:E:95:GLU:HG2	5:E:213:ILE:HG22	1.70	0.73
10:U:114:GLN:HE21	10:U:114:GLN:H	1.35	0.73
11:K:36:TYR:HE2	11:K:89:GLN:HG2	1.54	0.72
2:M:108:VAL:O	2:M:112:THR:HG23	1.87	0.72
3:C:58:ILE:H	3:C:173:ASN:HD22	1.36	0.72
2:B:62:ARG:HG2	2:B:62:ARG:HH21	1.54	0.71
1:L:32:LEU:HG	1:L:216:HIS:HE2	1.54	0.71
7:R:77:ARG:HD2	24:R:5803:HOH:O	1.91	0.70
3:N:253:HIS:HD2	3:N:255:ASP:H	1.38	0.70
5:P:115:PRO:HD2	5:P:158:ILE:HD11	1.73	0.70
1:L:404:GLY:HA2	2:M:27:LYS:HE3	1.72	0.70
11:K:6:GLN:HG2	11:K:23:CYS:SG	2.31	0.70
1:L:179:ARG:HH21	1:L:179:ARG:HG2	1.55	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:283:GLN:NE2	1:L:373:GLN:HE21	1.90	0.70
2:M:324:LYS:O	2:M:327:VAL:HG22	1.93	0.69
2:B:260:LEU:HD22	2:B:267:LEU:HD11	1.72	0.69
7:G:125:VAL:HG21	1:L:364:GLU:HG3	1.73	0.69
3:C:312:VAL:HG21	7:G:5:PHE:CE1	2.28	0.68
3:C:253:HIS:HD2	3:C:255:ASP:H	1.41	0.68
3:N:323:LYS:NZ	8:S:55:GLN:HE22	1.91	0.68
2:B:62:ARG:NH2	2:B:67:LEU:HD13	2.08	0.67
11:V:2:ILE:H	11:V:2:ILE:HD12	1.59	0.67
2:M:238:VAL:HG13	2:M:356:VAL:HB	1.75	0.67
5:P:172:ASP:H	5:P:184:HIS:CD2	2.11	0.67
1:A:156:HIS:HD2	1:A:159:ARG:HH21	1.42	0.67
2:M:300:ASN:O	2:M:304:ILE:HG12	1.95	0.66
2:B:300:ASN:O	2:B:304:ILE:HG12	1.95	0.66
2:M:260:LEU:HD22	2:M:267:LEU:HD11	1.78	0.66
4:D:227:ARG:HH11	4:D:244:THR:HG21	1.59	0.66
1:L:117:LEU:HD11	1:L:219:LEU:HD12	1.76	0.66
3:N:44:ILE:O	3:N:48:ILE:HG12	1.94	0.66
1:L:317:HIS:CE1	1:L:351:TRP:HE1	2.13	0.66
12:W:65:ASP:H	12:W:68:ASN:HD21	1.44	0.66
1:A:317:HIS:CE1	1:A:351:TRP:HE1	2.13	0.65
11:V:36:TYR:HE2	11:V:89:GLN:HG2	1.60	0.65
1:A:382:ASN:OD1	1:A:384:VAL:HG22	1.96	0.65
20:C:4033:CN5:H3CA	14:L:4113:6PH:H2E	1.79	0.65
1:L:58:GLY:H	1:L:61:ASN:HD22	1.45	0.65
1:L:207:VAL:HG11	1:L:394:VAL:HG21	1.80	0.64
2:B:49:HIS:CD2	2:B:161:TYR:H	2.14	0.64
2:M:31:LEU:HD12	2:M:105:LEU:HD12	1.79	0.64
3:C:320:VAL:HG23	24:C:7051:HOH:O	1.97	0.64
2:B:137:CYS:SG	24:B:8522:HOH:O	2.55	0.64
1:L:122:GLN:HA	1:L:126:GLN:HB3	1.79	0.63
2:M:247:LYS:O	2:M:250:LEU:HD22	1.98	0.63
1:L:72:LEU:HD23	1:L:193:LEU:HD21	1.80	0.63
5:P:91:MET:HG2	5:P:112:GLN:NE2	2.14	0.63
1:L:72:LEU:HB3	1:L:193:LEU:HD11	1.79	0.63
10:U:21:THR:HG22	10:U:80:PHE:HD2	1.63	0.63
1:A:68:GLY:HA3	1:A:185:LEU:HD11	1.81	0.63
1:L:72:LEU:HD22	1:L:188:LEU:HD23	1.79	0.62
2:B:164:VAL:HG21	2:M:232:ARG:HH11	1.63	0.62
4:O:213:ASN:OD1	13:O:4146:SUC:H6'2	1.99	0.62
4:D:113:ARG:HG2	4:D:151:LEU:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:134:MET:HG3	10:U:31:SER:HB3	1.81	0.62
5:E:48:ASP:HB3	5:E:51:LYS:HG2	1.80	0.62
5:E:172:ASP:H	5:E:184:HIS:HD2	1.47	0.62
3:C:208:ASN:HD22	3:C:210:LEU:H	1.47	0.62
4:O:113:ARG:NE	24:O:6841:HOH:O	2.27	0.62
2:B:146:LEU:O	2:B:150:THR:HG23	2.00	0.62
10:U:6:GLU:H	10:U:114:GLN:HE22	1.48	0.62
20:C:4033:CN5:H3E	14:L:4113:6PH:H2B	1.82	0.62
2:M:65:LEU:O	2:M:69:ARG:HG2	1.99	0.62
1:A:121:ASN:ND2	1:A:125:ILE:HD12	2.14	0.61
7:G:77:ARG:HD2	24:G:5303:HOH:O	1.99	0.61
3:C:27:ASN:HB2	22:D:4031:CN3:O2'	1.99	0.61
2:B:336:ILE:HD12	2:B:336:ILE:H	1.64	0.61
1:A:117:LEU:HD11	1:A:219:LEU:HD12	1.83	0.61
4:D:203:PRO:HG2	4:D:206:VAL:HG21	1.82	0.61
9:T:5:SER:O	9:T:9:THR:HG23	2.01	0.61
3:N:253:HIS:CD2	3:N:255:ASP:H	2.17	0.60
3:N:208:ASN:HD22	3:N:210:LEU:H	1.49	0.60
10:U:29:ILE:HG12	10:U:77:ASN:ND2	2.16	0.60
3:N:320:VAL:HG23	24:N:6971:HOH:O	2.02	0.60
10:J:28:SER:HB3	10:J:31:SER:OG	2.02	0.60
12:W:54:THR:CG2	12:W:84:LYS:HG3	2.31	0.60
1:A:72:LEU:HD23	1:A:193:LEU:HD21	1.83	0.60
3:N:58:ILE:H	3:N:173:ASN:ND2	1.99	0.59
9:T:8:LYS:O	9:T:12:LYS:HD2	2.02	0.59
2:M:71:SER:HA	2:M:74:LEU:CD1	2.32	0.59
3:C:4:ARG:HE	3:C:14:ASN:ND2	2.00	0.59
10:J:29:ILE:HG12	10:J:77:ASN:ND2	2.18	0.59
8:H:61:ILE:HB	8:H:62:PRO:HD3	1.83	0.59
3:C:52:MET:CE	5:E:82:MET:HG2	2.32	0.59
13:O:4146:SUC:C1'	12:W:20:LEU:HD23	2.31	0.59
3:N:27:ASN:HB2	22:N:4131:CN3:O2'	2.02	0.59
11:V:79:GLU:HB3	11:V:80:PRO:HD3	1.84	0.59
1:L:72:LEU:CD1	1:L:144:VAL:HG21	2.33	0.59
2:B:193:VAL:HG23	2:B:196:ASP:HB2	1.85	0.59
1:A:179:ARG:NH2	1:A:179:ARG:HG2	2.14	0.59
2:B:30:THR:CG2	2:B:190:GLU:HB3	2.33	0.59
1:L:252:ARG:HD3	1:L:254:ASP:OD1	2.03	0.59
4:D:227:ARG:NH1	4:D:244:THR:HG21	2.18	0.58
10:J:24:VAL:HG21	10:J:29:ILE:HD11	1.85	0.58
10:J:29:ILE:H	10:J:77:ASN:ND2	1.94	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:S:83:LYS:O	8:S:86:ARG:HG2	2.04	0.58
1:L:241:LYS:HD2	1:L:241:LYS:H	1.68	0.58
1:A:217:GLU:HA	1:A:220:VAL:HG12	1.86	0.58
1:A:228:LEU:HG	1:A:229:SER:H	1.67	0.58
2:B:121:GLU:OE2	7:R:62:ARG:HD2	2.04	0.58
8:H:56:PHE:O	8:H:60:LEU:HB2	2.03	0.58
1:L:156:HIS:HD2	1:L:159:ARG:HH21	1.51	0.58
3:C:253:HIS:CD2	3:C:255:ASP:H	2.21	0.58
6:F:77:GLN:HE21	6:F:77:GLN:N	1.93	0.58
3:C:214:GLY:O	3:C:218:ARG:HD2	2.03	0.58
1:A:283:GLN:HE22	1:A:373:GLN:HE21	1.52	0.58
4:D:247:MET:O	4:D:251:VAL:HG22	2.05	0.57
11:K:36:TYR:CE2	11:K:89:GLN:HG2	2.37	0.57
1:A:429:GLN:HE22	9:I:13:ARG:HH21	1.50	0.57
16:N:4022:HEM:HMC2	16:N:4022:HEM:HBC2	1.85	0.57
2:M:181:THR:HB	2:M:212:GLY:H	1.70	0.57
7:G:97:GLN:NE2	7:G:97:GLN:H	2.03	0.57
7:G:53:ASN:ND2	7:G:56:MET:H	2.03	0.57
2:B:315:SER:OG	2:B:344:LYS:HD2	2.04	0.57
7:G:63:LEU:HD12	7:G:64:PRO:HD2	1.87	0.56
7:G:91:ASN:H	7:G:91:ASN:ND2	2.02	0.56
10:J:114:GLN:H	10:J:114:GLN:NE2	1.96	0.56
2:B:117:HIS:HB3	7:R:62:ARG:HG2	1.88	0.56
1:A:283:GLN:NE2	1:A:373:GLN:HE21	2.03	0.56
1:L:110:PRO:HB3	1:L:213:ASN:HB3	1.87	0.56
2:M:49:HIS:CD2	2:M:161:TYR:H	2.20	0.56
2:M:110:TYR:CD2	2:M:205:LEU:HD23	2.41	0.56
2:B:347:LYS:N	2:B:347:LYS:HD3	2.20	0.56
2:M:35:VAL:CG1	2:M:179:VAL:HG12	2.36	0.56
2:B:164:VAL:CG2	2:M:232:ARG:HH11	2.18	0.56
5:P:103:LEU:O	5:P:120:HIS:HB3	2.06	0.56
3:N:313:VAL:HG22	3:N:319:LYS:HE3	1.87	0.56
2:B:53:ARG:HB3	2:B:123:VAL:HG13	1.89	0.55
10:U:61:ASN:HD22	10:U:63:SER:H	1.52	0.55
3:C:52:MET:HE1	5:E:82:MET:HG2	1.88	0.55
2:B:30:THR:HG22	2:B:190:GLU:HB3	1.87	0.55
3:C:313:VAL:HG22	3:C:319:LYS:HE3	1.88	0.55
1:L:270:VAL:O	1:L:271:ASN:HB2	2.05	0.55
15:A:4021:UMQ:HC1	9:I:18:VAL:HG12	1.88	0.55
1:A:58:GLY:H	1:A:61:ASN:ND2	2.02	0.55
22:D:4031:CN3:HAA	7:G:85:HIS:CE1	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:20:LEU:HD22	10:J:116:THR:HG21	1.89	0.55
10:J:65:LYS:HA	10:J:68:LEU:HD11	1.87	0.55
10:U:29:ILE:H	10:U:77:ASN:ND2	2.02	0.55
3:N:4:ARG:HE	3:N:14:ASN:ND2	2.04	0.55
13:O:4146:SUC:H1'2	12:W:20:LEU:CD2	2.34	0.55
5:E:172:ASP:H	5:E:184:HIS:CD2	2.25	0.55
5:P:72:LYS:NZ	9:T:29:GLN:HE22	2.04	0.55
11:V:29:ILE:HG22	11:V:92:ILE:HD12	1.88	0.55
3:N:57:ASN:HA	3:N:173:ASN:HD21	1.71	0.55
5:P:103:LEU:HG	5:P:122:THR:HG22	1.88	0.55
2:M:193:VAL:HG23	2:M:196:ASP:HB2	1.88	0.55
5:P:72:LYS:HZ3	9:T:29:GLN:HE22	1.55	0.54
5:P:91:MET:HG2	5:P:112:GLN:HE21	1.70	0.54
5:E:51:LYS:HD3	9:I:4:SER:HB2	1.88	0.54
3:N:323:LYS:CE	8:S:55:GLN:HE22	2.21	0.54
7:R:53:ASN:ND2	7:R:56:MET:H	2.05	0.54
11:V:37:GLN:HB2	11:V:47:LEU:HD11	1.89	0.54
1:L:169:PHE:O	1:L:172:THR:HB	2.08	0.54
10:J:21:THR:HG22	10:J:80:PHE:HD2	1.73	0.54
11:K:55:HIS:O	11:K:58:VAL:HG22	2.08	0.54
6:Q:81:LEU:HB3	6:Q:138:THR:HG22	1.89	0.54
2:B:44:LYS:O	2:B:47:VAL:HG23	2.07	0.54
3:N:147:ILE:HA	3:N:150:LEU:HD22	1.90	0.54
2:B:336:ILE:HG21	2:B:339:ASN:HD22	1.73	0.54
3:N:208:ASN:HB2	3:N:209:PRO:HD2	1.91	0.53
3:C:58:ILE:H	3:C:173:ASN:ND2	2.05	0.53
1:L:179:ARG:NH2	1:L:179:ARG:HG2	2.23	0.53
11:V:55:HIS:O	11:V:58:VAL:HG22	2.09	0.53
1:L:67:ASN:HD21	1:L:177:PRO:HG2	1.74	0.53
1:L:313:ASP:OD1	1:L:335:ARG:HD3	2.09	0.53
1:A:164:LEU:HD13	1:A:327:LEU:HD13	1.91	0.53
5:E:213:ILE:HG13	5:E:213:ILE:O	2.08	0.53
7:R:63:LEU:HD12	7:R:64:PRO:HD2	1.91	0.53
3:C:32:MET:HE2	3:C:95:MET:SD	2.48	0.53
2:M:71:SER:HA	2:M:74:LEU:HD11	1.89	0.53
7:G:62:ARG:HD2	2:M:121:GLU:OE2	2.08	0.53
8:S:89:LEU:O	8:S:93:ASN:HB2	2.08	0.53
1:L:382:ASN:OD1	1:L:384:VAL:HG22	2.08	0.53
1:A:207:VAL:HG11	1:A:394:VAL:HG21	1.90	0.53
1:A:302:LEU:HB2	1:A:350:GLN:HG3	1.91	0.53
10:U:14:PRO:O	10:U:15:SER:HB3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:53:ARG:HB3	2:M:123:VAL:HG13	1.89	0.53
2:M:255:VAL:HG11	2:M:343:VAL:HG21	1.91	0.53
12:W:104:LYS:O	12:W:108:GLU:HG2	2.08	0.53
1:L:130:ASN:HD22	1:L:130:ASN:H	1.57	0.53
4:O:286:TRP:CE3	5:P:59:MET:HG3	2.44	0.53
2:M:251:ALA:HB2	2:M:339:ASN:HB2	1.91	0.53
2:M:255:VAL:HG23	2:M:314:LEU:HD13	1.91	0.53
3:C:208:ASN:HB2	3:C:209:PRO:HD2	1.90	0.53
2:M:292:GLN:NE2	2:M:292:GLN:H	2.06	0.53
2:M:246:ASN:ND2	2:M:246:ASN:N	2.52	0.52
2:B:238:VAL:CG1	2:B:356:VAL:HB	2.36	0.52
3:N:184:TYR:CD1	16:N:4021:HEM:HBC1	2.44	0.52
10:U:87:THR:HG22	10:U:88:THR:N	2.24	0.52
8:S:61:ILE:HB	8:S:62:PRO:HD3	1.91	0.52
10:U:61:ASN:ND2	10:U:63:SER:H	2.06	0.52
2:M:146:LEU:O	2:M:150:THR:HG23	2.09	0.52
5:E:115:PRO:HD2	5:E:158:ILE:HD11	1.90	0.52
2:B:65:LEU:HD11	2:B:69:ARG:NH2	2.23	0.52
1:L:306:ILE:HA	1:L:311:LEU:HD22	1.92	0.52
2:B:35:VAL:CG1	2:B:179:VAL:HG12	2.39	0.52
2:M:238:VAL:CG1	2:M:356:VAL:HB	2.39	0.52
1:A:350:GLN:HE22	1:A:353:ARG:HH21	1.57	0.52
11:V:34:ASN:HD22	11:V:49:TYR:HA	1.75	0.52
6:Q:77:GLN:N	6:Q:77:GLN:HE21	1.94	0.52
7:G:81:THR:HG22	7:G:86:HIS:O	2.10	0.52
4:O:78:HIS:HD2	24:O:5586:HOH:O	1.91	0.52
2:B:311:GLY:O	2:B:312:LYS:HD2	2.09	0.52
1:L:66:ASN:HA	1:L:188:LEU:HD11	1.90	0.52
2:M:106:ALA:HA	2:M:206:LEU:HD13	1.92	0.52
1:L:289:ASN:HD22	1:L:289:ASN:C	2.12	0.52
1:L:76:ILE:HG23	1:L:140:THR:HG21	1.92	0.52
2:M:68:VAL:O	2:M:72:GLU:HG3	2.10	0.52
1:L:344:ILE:HG21	1:L:448:ILE:HD12	1.91	0.52
2:M:146:LEU:HD23	2:M:286:THR:HG22	1.91	0.52
7:G:117:LYS:HE2	24:M:7272:HOH:O	2.09	0.52
2:M:31:LEU:HD12	2:M:105:LEU:CD1	2.40	0.52
1:L:28:GLU:HG2	1:L:29:VAL:N	2.25	0.52
11:K:15:LEU:H	11:K:15:LEU:HD12	1.75	0.52
12:W:68:ASN:HD22	12:W:69:MET:N	2.08	0.51
1:A:145:LEU:CD1	1:A:185:LEU:HB3	2.40	0.51
3:C:4:ARG:HE	3:C:14:ASN:HD21	1.56	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:147:ILE:O	3:C:150:LEU:HB2	2.09	0.51
3:N:222:HIS:O	3:N:223:SER:HB2	2.10	0.51
1:L:181:THR:O	1:L:185:LEU:HB2	2.09	0.51
4:D:286:TRP:CZ3	5:E:56:ALA:HA	2.45	0.51
6:Q:117:LEU:O	6:Q:118:GLU:HG2	2.09	0.51
10:U:4:LEU:HG	10:U:24:VAL:HG22	1.91	0.51
21:D:4014:7PH:H35	5:E:70:GLY:HA3	1.93	0.51
7:G:13:ASP:HB3	7:G:17:LYS:HE3	1.93	0.51
3:N:310:ARG:HA	7:R:2:PRO:HB2	1.92	0.51
1:L:172:THR:CG2	1:L:242:ALA:HA	2.41	0.51
3:N:63:SER:OG	4:O:109:ARG:NH1	2.43	0.51
7:G:91:ASN:H	7:G:91:ASN:HD22	1.58	0.51
1:L:28:GLU:HG2	1:L:29:VAL:H	1.74	0.51
10:J:114:GLN:HE21	10:J:114:GLN:N	2.00	0.51
1:L:283:GLN:HE21	1:L:373:GLN:HE21	1.58	0.51
4:D:231:ASP:OD1	4:D:244:THR:HG23	2.10	0.51
4:D:225:MET:HB2	16:D:4003:HEM:C1D	2.46	0.50
1:A:430:ASP:OD2	1:A:449:ARG:NH2	2.44	0.50
8:S:52:PHE:O	8:S:56:PHE:HB3	2.12	0.50
20:C:4033:CN5:H1'A	20:C:4033:CN5:HB	1.92	0.50
1:L:240:LYS:HG2	1:L:241:LYS:N	2.26	0.50
2:M:261:THR:O	2:M:261:THR:HG22	2.11	0.50
5:P:122:THR:O	5:P:126:ILE:HG13	2.10	0.50
1:L:67:ASN:HD22	1:L:181:THR:HG23	1.76	0.50
7:G:62:ARG:HG2	2:M:117:HIS:HB3	1.92	0.50
1:A:313:ASP:OD1	1:A:335:ARG:HD3	2.12	0.50
4:O:289:LYS:HB2	8:S:37:LEU:HD13	1.92	0.50
10:J:49:VAL:CG1	10:J:68:LEU:HD23	2.42	0.50
10:U:38:ILE:HD12	10:U:46:LEU:HD22	1.92	0.50
10:U:61:ASN:C	10:U:61:ASN:HD22	2.15	0.50
3:C:79:ARG:NH1	24:C:6790:HOH:O	2.45	0.50
15:L:4121:UMQ:O1'	9:T:18:VAL:HG13	2.11	0.50
1:A:252:ARG:HD3	1:A:254:ASP:OD1	2.12	0.50
3:C:235:LEU:HD23	22:D:4031:CN3:H45	1.93	0.50
2:B:112:THR:HG22	24:B:6011:HOH:O	2.12	0.50
5:E:103:LEU:O	5:E:120:HIS:HB3	2.12	0.50
11:K:29:ILE:HD11	11:K:71:TYR:CE1	2.47	0.50
10:U:114:GLN:H	10:U:114:GLN:NE2	2.07	0.50
1:A:67:ASN:HD21	1:A:177:PRO:HG2	1.75	0.50
22:N:4131:CN3:HC	24:O:6998:HOH:O	2.12	0.49
7:G:12:GLY:O	7:G:16:LEU:HD22	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:241:LYS:H	1:L:241:LYS:CD	2.25	0.49
21:O:4114:7PH:H35	5:P:70:GLY:HA3	1.94	0.49
8:S:42:HIS:H	8:S:45:VAL:HG12	1.76	0.49
1:L:265:VAL:HG21	1:L:426:LEU:HD12	1.93	0.49
2:B:146:LEU:HD13	2:B:354:VAL:HG22	1.94	0.49
10:J:61:ASN:C	10:J:61:ASN:HD22	2.16	0.49
11:K:2:ILE:HD11	11:K:93:LYS:NZ	2.28	0.49
1:L:172:THR:HG23	1:L:242:ALA:HA	1.95	0.49
5:E:168:GLY:HA2	5:E:176:TRP:CD1	2.47	0.49
4:D:286:TRP:CE3	5:E:59:MET:HG3	2.47	0.49
15:L:4121:UMQ:HC1	9:T:18:VAL:HG12	1.94	0.49
2:M:260:LEU:CD2	2:M:267:LEU:HD11	2.42	0.49
3:N:4:ARG:HE	3:N:14:ASN:HD21	1.58	0.49
3:N:147:ILE:O	3:N:150:LEU:HB2	2.13	0.49
1:A:67:ASN:HD22	1:A:181:THR:HG23	1.77	0.49
11:K:2:ILE:HD12	11:K:2:ILE:N	2.27	0.49
1:L:270:VAL:HG21	1:L:396:ILE:HD13	1.94	0.49
1:A:297:LEU:O	2:B:69:ARG:NH2	2.40	0.49
1:A:229:SER:HB3	1:A:232:THR:HB	1.95	0.49
11:K:31:ASN:ND2	11:K:51:THR:HG21	2.21	0.48
10:J:37:TRP:O	10:J:49:VAL:HB	2.13	0.48
4:D:109:ARG:NH2	24:D:6205:HOH:O	2.46	0.48
1:A:48:THR:HG21	2:B:327:VAL:HG12	1.95	0.48
11:K:34:ASN:HD22	11:K:49:TYR:HA	1.76	0.48
11:K:2:ILE:H	11:K:2:ILE:HD12	1.78	0.48
4:D:78:HIS:HD2	24:D:5086:HOH:O	1.96	0.48
1:A:289:ASN:HD22	1:A:289:ASN:C	2.16	0.48
4:O:203:PRO:HG2	4:O:206:VAL:HG21	1.94	0.48
1:A:68:GLY:HA3	1:A:185:LEU:CD1	2.42	0.48
3:C:222:HIS:O	3:C:223:SER:HB2	2.12	0.48
11:V:17:ASP:O	11:V:78:LEU:HD13	2.14	0.48
11:V:53:ARG:HH21	11:V:53:ARG:HG3	1.77	0.48
11:V:47:LEU:HA	11:V:58:VAL:HG11	1.96	0.48
1:A:250:ARG:NH1	1:A:442:LEU:O	2.47	0.48
12:W:92:LYS:HD2	12:W:94:LYS:HE2	1.95	0.48
12:W:60:LYS:HG2	12:W:80:ILE:HG12	1.94	0.48
7:R:120:LEU:HA	7:R:123:ILE:HG23	1.94	0.48
5:E:93:LYS:HD3	5:E:215:GLY:HA3	1.95	0.48
10:J:29:ILE:N	10:J:77:ASN:HD21	1.98	0.48
11:V:19:VAL:HG12	11:V:75:ILE:HB	1.96	0.48
2:B:318:ILE:HG22	24:B:8526:HOH:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:318:ILE:CD1	2:B:340:PHE:HB3	2.39	0.48
11:K:18:ARG:HB2	11:K:75:ILE:O	2.14	0.48
5:P:125:GLU:HB3	5:P:187:ILE:HG12	1.95	0.48
1:L:250:ARG:NH1	1:L:442:LEU:O	2.47	0.48
1:A:252:ARG:HD2	8:H:21:GLN:HB2	1.94	0.47
5:P:214:VAL:N	24:P:7409:HOH:O	2.46	0.47
5:P:65:LEU:HD13	9:T:25:ALA:HA	1.96	0.47
1:L:66:ASN:HD22	1:L:66:ASN:H	1.63	0.47
3:N:332:ASN:HD21	3:N:355:ALA:HA	1.78	0.47
4:O:213:ASN:HB3	13:O:4146:SUC:O4	2.14	0.47
10:J:61:ASN:HD22	10:J:62:PRO:N	2.12	0.47
3:C:184:TYR:CD1	16:C:4001:HEM:HBC1	2.49	0.47
11:V:50:TYR:O	11:V:51:THR:HG22	2.13	0.47
20:C:4033:CN5:H3FB	14:L:4113:6PH:H29A	1.96	0.47
10:J:61:ASN:ND2	10:J:63:SER:H	2.13	0.47
4:D:203:PRO:HG2	4:D:206:VAL:CG2	2.43	0.47
5:P:94:VAL:N	24:P:7409:HOH:O	2.46	0.47
5:E:112:GLN:O	5:E:114:LYS:HD3	2.14	0.47
11:V:34:ASN:ND2	11:V:49:TYR:HA	2.29	0.47
3:C:147:ILE:HA	3:C:150:LEU:HD22	1.96	0.47
2:B:40:ARG:HG3	2:B:155:LEU:HG	1.95	0.47
9:T:50:LYS:HG3	24:T:6999:HOH:O	2.13	0.47
2:B:106:ALA:HA	2:B:206:LEU:HD13	1.96	0.47
3:C:323:LYS:HE3	8:H:55:GLN:HE22	1.80	0.47
10:U:36:ASN:OD1	10:U:51:TYR:HB3	2.15	0.47
6:Q:92:LYS:HA	6:Q:95:VAL:HG22	1.96	0.47
11:K:90:HIS:HD2	11:K:92:ILE:HG22	1.80	0.47
11:K:21:ILE:HG22	11:K:22:SER:N	2.30	0.47
2:M:230:ARG:HE	2:M:359:VAL:HG13	1.80	0.47
1:L:172:THR:HG23	1:L:173:PRO:HD2	1.97	0.47
2:B:324:LYS:O	2:B:327:VAL:HG22	2.14	0.47
11:K:34:ASN:HD21	11:K:91:HIS:HE1	1.63	0.47
10:J:51:TYR:C	10:J:51:TYR:CD2	2.89	0.47
4:D:268:ARG:NH1	9:I:33:ASP:OD1	2.48	0.47
1:L:164:LEU:HD13	1:L:327:LEU:HD13	1.97	0.47
2:B:139:VAL:HG22	24:B:8522:HOH:O	2.15	0.47
11:V:19:VAL:HG12	11:V:78:LEU:HD11	1.97	0.47
5:E:132:VAL:HG21	5:E:192:ARG:NH1	2.30	0.47
4:D:69:LEU:HD11	6:F:131:GLN:HB3	1.96	0.47
5:P:43:LEU:HD21	8:S:29:VAL:HG11	1.97	0.47
2:B:152:ARG:HD3	2:B:224:PHE:CE1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:143:GLY:O	3:C:147:ILE:HG12	2.15	0.46
9:I:3:PHE:CE1	9:I:5:SER:HB2	2.50	0.46
10:J:48:TRP:CZ2	10:J:50:GLY:HA2	2.50	0.46
2:B:49:HIS:HA	2:B:82:LEU:HD22	1.98	0.46
5:P:65:LEU:CD1	9:T:25:ALA:HA	2.45	0.46
2:B:205:LEU:HD23	24:B:7883:HOH:O	2.16	0.46
3:C:77:ILE:O	3:C:81:LEU:HB2	2.15	0.46
5:E:43:LEU:HD21	8:H:29:VAL:HG11	1.97	0.46
4:D:296:LYS:HE3	24:D:5128:HOH:O	2.15	0.46
4:O:134:TYR:OH	4:O:156:PRO:HD3	2.16	0.46
2:M:228:GLU:HA	2:M:353:TYR:O	2.15	0.46
2:M:89:LEU:HD12	2:M:89:LEU:N	2.31	0.46
11:V:93:LYS:HB3	11:V:93:LYS:NZ	2.30	0.46
2:M:315:SER:O	2:M:318:ILE:HG22	2.15	0.46
4:D:113:ARG:NH1	24:D:5360:HOH:O	2.48	0.46
1:A:283:GLN:NE2	1:A:373:GLN:NE2	2.63	0.46
22:N:4131:CN3:HAA	7:R:85:HIS:CE1	2.51	0.46
3:C:57:ASN:HA	3:C:173:ASN:HD21	1.80	0.46
1:A:156:HIS:HD2	1:A:159:ARG:NH2	2.13	0.46
10:U:61:ASN:HD22	10:U:62:PRO:N	2.13	0.46
21:O:4114:7PH:H25	21:O:4114:7PH:H2AA	1.97	0.46
5:E:45:GLU:HB3	5:E:47:ASN:ND2	2.31	0.46
3:C:142:TRP:CH2	5:P:165:VAL:HG23	2.51	0.46
20:C:4033:CN5:H2A	3:N:199:MET:HG2	1.97	0.46
8:S:35:LYS:O	8:S:37:LEU:N	2.49	0.45
1:L:283:GLN:NE2	1:L:373:GLN:NE2	2.63	0.45
2:B:44:LYS:HB2	2:B:47:VAL:CG2	2.47	0.45
5:E:55:TYR:O	5:E:59:MET:HG2	2.16	0.45
2:M:84:ARG:HD2	2:M:159:LEU:HD13	1.99	0.45
1:A:66:ASN:H	1:A:66:ASN:HD22	1.65	0.45
2:B:35:VAL:HG12	2:B:179:VAL:HG12	1.99	0.45
1:L:207:VAL:HG11	1:L:394:VAL:CG2	2.45	0.45
1:L:130:ASN:HD22	1:L:130:ASN:N	2.14	0.45
4:O:286:TRP:CZ3	5:P:56:ALA:HA	2.51	0.45
3:N:203:ILE:HB	8:S:8:THR:HG21	1.98	0.45
3:C:32:MET:HE3	3:C:92:VAL:HG13	1.99	0.45
1:L:289:ASN:ND2	1:L:291:PHE:H	2.14	0.45
2:B:152:ARG:HD2	24:B:8523:HOH:O	2.17	0.45
2:B:68:VAL:O	2:B:72:GLU:HG3	2.17	0.45
2:B:69:ARG:NH1	7:R:121:ASP:OD1	2.49	0.45
4:D:286:TRP:CD2	5:E:59:MET:HG3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:LYS:HE2	2:B:263:ALA:HA	1.97	0.45
2:M:146:LEU:HD13	2:M:354:VAL:HG22	1.99	0.45
10:U:21:THR:HG22	10:U:80:PHE:CD2	2.49	0.45
1:L:67:ASN:ND2	1:L:181:THR:HG23	2.31	0.45
1:L:47:HIS:CE1	2:M:22:ARG:HH22	2.35	0.45
2:M:71:SER:HA	2:M:74:LEU:HD12	1.99	0.45
2:B:193:VAL:HG22	24:B:7468:HOH:O	2.15	0.45
10:U:37:TRP:CZ3	10:U:96:CYS:HB3	2.52	0.45
2:M:74:LEU:HD13	2:M:101:TYR:OH	2.18	0.44
3:C:95:MET:HG2	18:C:4010:8PE:H37A	1.99	0.44
3:N:18:ILE:HA	3:N:222:HIS:HB2	1.99	0.44
11:K:14:SER:HB2	11:K:17:ASP:OD2	2.17	0.44
3:C:48:ILE:HD13	3:N:185:LEU:HG	1.98	0.44
8:H:3:PRO:HG3	8:S:12:TRP:CE2	2.52	0.44
2:M:52:ASN:HD22	2:M:87:ILE:HG23	1.82	0.44
5:P:168:GLY:HA2	5:P:176:TRP:CD1	2.52	0.44
1:L:37:VAL:HG13	1:L:207:VAL:HA	2.00	0.44
2:M:44:LYS:HB2	2:M:47:VAL:CG2	2.47	0.44
3:N:216:LEU:HD12	3:N:216:LEU:N	2.33	0.44
1:L:184:SER:O	1:L:188:LEU:HD13	2.17	0.44
15:A:4021:UMQ:O1'	9:I:18:VAL:HG13	2.17	0.44
7:G:18:SER:OG	7:G:21:LEU:HD23	2.17	0.44
1:L:57:SER:O	1:L:102:GLN:HB2	2.18	0.44
2:B:318:ILE:HD13	2:B:343:VAL:HG22	1.99	0.44
1:A:60:ALA:O	1:A:173:PRO:HB3	2.17	0.44
5:E:208:ASP:O	5:E:211:LYS:HG2	2.17	0.44
1:A:39:ALA:HB1	1:A:390:LEU:HD11	1.99	0.44
7:R:80:GLN:O	7:R:84:THR:HG23	2.17	0.44
1:L:58:GLY:H	1:L:61:ASN:ND2	2.14	0.44
1:A:121:ASN:HD22	1:A:125:ILE:HD12	1.81	0.44
3:C:32:MET:CE	3:C:92:VAL:HG13	2.46	0.44
1:L:73:TRP:HA	1:L:76:ILE:HD11	1.99	0.44
10:J:21:THR:HG22	10:J:80:PHE:CD2	2.52	0.44
11:K:34:ASN:ND2	11:K:50:TYR:H	2.16	0.44
10:J:87:THR:HG22	10:J:88:THR:N	2.32	0.44
2:B:66:LYS:O	2:B:70:GLU:HB2	2.18	0.44
1:A:72:LEU:HD13	1:A:144:VAL:HG21	2.00	0.44
10:J:107:TYR:H	11:K:91:HIS:CD2	2.36	0.44
12:W:46:GLY:HA2	12:W:53:TYR:CE1	2.53	0.44
4:O:136:ASP:HB3	4:O:145:LYS:HG3	2.00	0.44
1:A:270:VAL:HG21	1:A:396:ILE:HD13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:173:ASN:HB3	3:N:174:PRO:HD3	2.00	0.44
11:K:15:LEU:N	11:K:15:LEU:HD12	2.33	0.44
11:K:90:HIS:CD2	11:K:92:ILE:HG22	2.52	0.44
5:E:45:GLU:HG2	5:E:46:ASN:H	1.81	0.44
1:A:69:VAL:HG23	1:A:193:LEU:HD22	2.00	0.43
4:O:286:TRP:CD2	5:P:59:MET:HG3	2.53	0.43
1:A:169:PHE:O	1:A:175:SER:HB3	2.18	0.43
10:J:40:LEU:HB3	10:J:93:THR:OG1	2.18	0.43
1:A:380:SER:HB3	24:A:7013:HOH:O	2.17	0.43
1:L:349:LYS:HA	1:L:349:LYS:HE2	2.00	0.43
11:K:34:ASN:ND2	11:K:49:TYR:HA	2.33	0.43
1:A:172:THR:CG2	1:A:242:ALA:HA	2.48	0.43
1:A:152:GLU:HG3	24:A:6944:HOH:O	2.18	0.43
3:N:76:TYR:CG	4:O:262:GLU:HG3	2.53	0.43
5:E:106:ASN:ND2	5:E:119:ARG:HB2	2.33	0.43
8:H:35:LYS:O	8:H:37:LEU:N	2.46	0.43
11:V:6:GLN:HG2	11:V:23:CYS:SG	2.58	0.43
1:L:72:LEU:HD12	1:L:72:LEU:HA	1.88	0.43
2:B:62:ARG:HH21	2:B:62:ARG:CG	2.27	0.43
2:B:315:SER:HB2	2:B:316:PRO:HD3	2.00	0.43
4:D:277:LEU:HD21	21:D:4014:7PH:H34	2.00	0.43
5:E:72:LYS:NZ	9:I:29:GLN:HE22	2.16	0.43
10:J:13:GLN:HA	10:J:121:SER:O	2.18	0.43
2:M:124:LEU:HB3	2:M:128:ARG:NH2	2.33	0.43
1:L:430:ASP:OD2	1:L:449:ARG:NH2	2.48	0.43
7:G:120:LEU:HA	7:G:123:ILE:HG23	2.01	0.43
1:A:169:PHE:O	1:A:172:THR:HB	2.19	0.43
12:W:65:ASP:H	12:W:68:ASN:ND2	2.14	0.43
5:P:187:ILE:O	5:P:187:ILE:HG13	2.19	0.43
8:S:48:SER:O	8:S:49:PHE:HB2	2.18	0.43
11:V:27:GLN:HG2	11:V:28:ASP:N	2.34	0.43
22:D:4031:CN3:HC	24:D:6590:HOH:O	2.19	0.43
1:L:252:ARG:HD2	8:S:21:GLN:HB2	2.00	0.43
1:A:38:VAL:HA	1:A:208:VAL:HG13	2.01	0.43
12:W:10:LYS:NZ	12:W:10:LYS:HB2	2.33	0.43
1:L:227:ASN:N	1:L:227:ASN:HD22	2.17	0.43
2:M:318:ILE:HG23	2:M:319:ASN:N	2.34	0.43
5:P:65:LEU:HD12	5:P:65:LEU:C	2.40	0.43
10:U:51:TYR:CD2	10:U:51:TYR:C	2.92	0.43
11:K:92:ILE:O	11:K:92:ILE:HD13	2.18	0.43
3:C:362:TYR:O	3:C:367:VAL:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:123:GLU:H	4:D:123:GLU:CD	2.21	0.43
3:N:58:ILE:HB	3:N:173:ASN:HA	2.01	0.43
3:C:312:VAL:HG21	7:G:5:PHE:CZ	2.53	0.43
10:J:49:VAL:HG12	10:J:68:LEU:HD23	2.01	0.43
1:L:62:GLU:OE1	1:L:67:ASN:HA	2.18	0.43
2:M:292:GLN:H	2:M:292:GLN:CD	2.22	0.43
8:S:47:ASN:O	8:S:50:ARG:HB3	2.19	0.43
11:K:63:SER:HB2	11:K:74:THR:HB	2.01	0.43
2:B:146:LEU:HA	2:B:146:LEU:HD12	1.87	0.42
2:M:251:ALA:CB	2:M:339:ASN:HB2	2.49	0.42
10:U:38:ILE:CD1	10:U:46:LEU:HD22	2.49	0.42
2:M:317:ALA:O	2:M:321:THR:HG22	2.18	0.42
5:E:103:LEU:O	5:E:120:HIS:O	2.37	0.42
11:V:31:ASN:HD22	11:V:51:THR:HG21	1.84	0.42
2:B:152:ARG:HG2	2:M:364:TYR:CZ	2.55	0.42
8:H:41:PHE:O	8:H:42:HIS:HB3	2.19	0.42
3:C:216:LEU:HD12	3:C:216:LEU:N	2.34	0.42
3:C:173:ASN:HB3	3:C:174:PRO:HD3	2.01	0.42
1:L:127:GLN:HB3	1:L:130:ASN:ND2	2.34	0.42
3:C:25:SER:OG	7:G:79:HIS:HD2	2.02	0.42
11:V:2:ILE:N	11:V:2:ILE:HD12	2.29	0.42
5:P:203:PRO:O	5:P:205:TYR:HD1	2.02	0.42
2:B:35:VAL:HG12	2:B:179:VAL:CG1	2.50	0.42
1:L:349:LYS:HE2	1:L:352:ASN:OD1	2.20	0.42
3:N:25:SER:OG	7:R:79:HIS:HD2	2.03	0.42
2:M:40:ARG:HA	2:M:154:GLY:O	2.19	0.42
3:N:157:VAL:O	3:N:161:ILE:HG12	2.20	0.42
4:D:301:VAL:CG2	8:H:25:THR:HB	2.50	0.42
1:L:235:LYS:NZ	1:L:235:LYS:HB2	2.35	0.42
2:M:59:THR:HA	2:M:112:THR:HA	2.02	0.42
10:U:34:TYR:HB2	10:U:99:SER:OG	2.20	0.42
3:N:77:ILE:O	3:N:81:LEU:HB2	2.19	0.42
10:J:24:VAL:CG2	10:J:29:ILE:HD11	2.49	0.42
22:N:4131:CN3:CC	24:O:6998:HOH:O	2.68	0.42
7:R:45:PHE:O	7:R:48:LEU:HB2	2.19	0.42
10:U:48:TRP:CZ2	10:U:50:GLY:HA2	2.54	0.42
1:L:209:VAL:HG13	1:L:390:LEU:HD13	2.02	0.42
10:U:98:ARG:O	10:U:109:MET:HA	2.19	0.42
2:B:141:SER:HB2	24:B:7070:HOH:O	2.19	0.42
3:N:165:LEU:O	3:N:178:ARG:HD2	2.20	0.42
3:N:301:VAL:O	3:N:304:VAL:HG22	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:P:85:THR:O	5:P:88:VAL:HG22	2.20	0.41
11:K:4:LEU:N	11:K:4:LEU:HD12	2.34	0.41
2:B:362:LEU:HD12	2:B:362:LEU:HA	1.90	0.41
1:A:74:LYS:HG3	1:A:95:SER:HB3	2.01	0.41
1:A:145:LEU:HD11	1:A:185:LEU:HB3	2.01	0.41
1:A:169:PHE:HB3	1:A:172:THR:HG22	2.02	0.41
2:B:230:ARG:NE	2:B:359:VAL:HG13	2.34	0.41
1:A:57:SER:O	1:A:102:GLN:HB2	2.20	0.41
2:M:98:LEU:N	2:M:99:PRO:HD2	2.35	0.41
2:B:255:VAL:HG23	2:B:314:LEU:HD13	2.02	0.41
4:O:296:LYS:HE3	24:O:5628:HOH:O	2.19	0.41
3:C:332:ASN:HD21	3:C:355:ALA:HA	1.85	0.41
2:M:112:THR:OG1	2:M:114:PHE:CE2	2.74	0.41
11:V:32:PHE:HB2	11:V:92:ILE:HG22	2.03	0.41
11:K:34:ASN:ND2	11:K:91:HIS:HE1	2.18	0.41
3:C:121:PHE:CZ	3:C:125:ILE:HD11	2.55	0.41
3:N:20:SER:HA	3:N:21:PRO:HD3	1.93	0.41
10:U:18:LEU:O	10:U:82:LYS:HA	2.20	0.41
14:A:4013:6PH:H38	3:C:230:LEU:HD11	2.02	0.41
11:V:15:LEU:N	11:V:15:LEU:HD12	2.34	0.41
3:C:117:GLY:O	16:C:4002:HEM:HMC3	2.21	0.41
3:N:48:ILE:HD12	3:N:184:TYR:OH	2.21	0.41
3:C:214:GLY:O	3:C:218:ARG:CD	2.69	0.41
11:V:53:ARG:NH2	11:V:53:ARG:HG3	2.35	0.41
8:S:48:SER:C	8:S:50:ARG:H	2.23	0.41
2:M:254:GLU:HG2	2:M:276:LEU:HD23	2.02	0.41
11:V:21:ILE:HG22	11:V:22:SER:N	2.35	0.41
1:L:115:LYS:HD2	1:L:115:LYS:HA	1.88	0.41
7:R:18:SER:OG	7:R:21:LEU:HD23	2.20	0.41
1:L:241:LYS:HD2	1:L:241:LYS:N	2.35	0.41
2:M:230:ARG:NE	2:M:359:VAL:HG13	2.35	0.41
1:A:172:THR:HG23	1:A:242:ALA:HA	2.03	0.41
10:J:76:LYS:HB2	10:J:78:GLN:HG2	2.02	0.41
3:N:166:TRP:CE3	3:N:170:SER:HA	2.54	0.41
2:M:312:LYS:HB3	2:M:312:LYS:HE2	1.75	0.41
2:B:193:VAL:O	2:B:193:VAL:HG23	2.21	0.41
1:L:289:ASN:HD22	1:L:291:PHE:H	1.69	0.41
3:C:147:ILE:HD12	17:C:4005:SMA:H14	2.02	0.41
8:S:49:PHE:O	8:S:53:LYS:HB2	2.21	0.41
2:B:230:ARG:HE	2:B:359:VAL:HG13	1.85	0.41
1:L:74:LYS:HG3	1:L:95:SER:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:165:VAL:HG23	3:N:142:TRP:CH2	2.56	0.41
11:K:48:ILE:HD13	11:K:54:LEU:HA	2.03	0.41
1:A:364:GLU:HG3	7:R:125:VAL:HG21	2.03	0.41
4:O:111:ALA:HA	4:O:154:TYR:HA	2.02	0.41
1:L:424:LYS:HA	1:L:424:LYS:HD2	1.94	0.41
11:V:2:ILE:H	11:V:2:ILE:CD1	2.32	0.41
8:H:2:GLY:HA2	8:H:3:PRO:HD3	1.83	0.41
7:R:91:ASN:HD22	7:R:91:ASN:H	1.69	0.41
2:B:336:ILE:HD12	2:B:336:ILE:N	2.35	0.40
11:K:4:LEU:HD23	11:K:88:CYS:SG	2.60	0.40
2:M:197:LEU:O	2:M:201:VAL:HG23	2.20	0.40
1:A:179:ARG:NH2	1:A:179:ARG:CG	2.81	0.40
16:N:4021:HEM:HHD	16:N:4021:HEM:HBC2	2.02	0.40
1:A:228:LEU:HG	1:A:229:SER:N	2.36	0.40
1:A:67:ASN:ND2	1:A:181:THR:HG23	2.35	0.40
2:M:50:LEU:HA	2:M:50:LEU:HD23	1.92	0.40
2:B:146:LEU:HG	2:B:242:GLY:HA3	2.03	0.40
2:B:112:THR:OG1	2:B:114:PHE:CE2	2.74	0.40
2:B:164:VAL:CG2	2:M:232:ARG:NH1	2.84	0.40
10:J:40:LEU:HB3	10:J:93:THR:HG1	1.87	0.40
3:C:104:GLY:HA2	3:C:106:TYR:CE2	2.56	0.40
5:E:106:ASN:HD21	5:E:119:ARG:HD2	1.86	0.40
11:V:33:LEU:HD13	11:V:71:TYR:CD1	2.55	0.40
1:L:43:ASN:HA	1:L:44:PRO:HD2	1.92	0.40
7:R:100:VAL:HG13	7:R:101:PRO:HD2	2.02	0.40
2:M:137:CYS:HA	2:M:138:PRO:HD2	1.93	0.40
8:S:7:LYS:HD3	8:S:7:LYS:HA	1.84	0.40
1:L:228:LEU:O	1:L:228:LEU:HD12	2.22	0.40
2:B:181:THR:HB	2:B:212:GLY:H	1.86	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%)	408 (95%)	19 (4%)	2 (0%)	34 21
1	L	429/431 (100%)	406 (95%)	19 (4%)	4 (1%)	21 9
2	B	350/352 (99%)	330 (94%)	15 (4%)	5 (1%)	14 4
2	M	350/352 (99%)	330 (94%)	19 (5%)	1 (0%)	46 35
3	C	383/385 (100%)	370 (97%)	12 (3%)	1 (0%)	46 35
3	N	383/385 (100%)	369 (96%)	13 (3%)	1 (0%)	46 35
4	D	246/248 (99%)	238 (97%)	8 (3%)	0	100 100
4	O	246/248 (99%)	241 (98%)	4 (2%)	1 (0%)	39 27
5	E	183/185 (99%)	173 (94%)	8 (4%)	2 (1%)	17 6
5	P	183/185 (99%)	169 (92%)	10 (6%)	4 (2%)	8 1
6	F	72/146 (49%)	71 (99%)	1 (1%)	0	100 100
6	Q	72/146 (49%)	70 (97%)	2 (3%)	0	100 100
7	G	124/126 (98%)	122 (98%)	2 (2%)	0	100 100
7	R	124/126 (98%)	123 (99%)	1 (1%)	0	100 100
8	H	91/93 (98%)	83 (91%)	7 (8%)	1 (1%)	17 6
8	S	91/93 (98%)	83 (91%)	7 (8%)	1 (1%)	17 6
9	I	55/65 (85%)	53 (96%)	2 (4%)	0	100 100
9	T	55/65 (85%)	52 (94%)	2 (4%)	1 (2%)	11 2
10	J	125/127 (98%)	114 (91%)	11 (9%)	0	100 100
10	U	125/127 (98%)	115 (92%)	10 (8%)	0	100 100
11	K	105/107 (98%)	91 (87%)	10 (10%)	4 (4%)	4 0
11	V	105/107 (98%)	91 (87%)	11 (10%)	3 (3%)	6 1
12	W	106/108 (98%)	104 (98%)	2 (2%)	0	100 100
All	All	4432/4638 (96%)	4206 (95%)	195 (4%)	31 (1%)	26 14

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	103	LEU
5	P	103	LEU
2	B	153	LYS
3	C	223	SER
1	L	228	LEU
3	N	223	SER
11	V	30	ASN

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Mol	Chain	Res	Type
1	A	128	LYS
2	B	335	PRO
11	K	51	THR
1	L	232	THR
2	M	342	ALA
4	O	308	ARG
8	S	36	PRO
9	T	13	ARG
2	B	337	GLU
8	H	36	PRO
1	L	34	ASN
5	P	209	GLY
1	A	29	VAL
2	B	332	VAL
2	B	339	ASN
5	E	46	ASN
1	L	227	ASN
5	P	47	ASN
5	P	102	PRO
11	V	51	THR
11	K	68	GLY
11	V	16	GLY
11	K	9	VAL
11	K	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%)	343 (93%)	27 (7%)	17 7
1	L	370/370 (100%)	340 (92%)	30 (8%)	15 5
2	B	301/301 (100%)	288 (96%)	13 (4%)	35 23
2	M	301/301 (100%)	282 (94%)	19 (6%)	22 10
3	C	338/338 (100%)	318 (94%)	20 (6%)	24 12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	N	338/338 (100%)	321 (95%)	17 (5%)	30 18
4	D	206/206 (100%)	200 (97%)	6 (3%)	50 40
4	O	206/206 (100%)	202 (98%)	4 (2%)	65 59
5	E	151/151 (100%)	149 (99%)	2 (1%)	76 73
5	P	151/151 (100%)	146 (97%)	5 (3%)	45 34
6	F	67/130 (52%)	62 (92%)	5 (8%)	17 7
6	Q	67/130 (52%)	63 (94%)	4 (6%)	24 12
7	G	110/110 (100%)	105 (96%)	5 (4%)	34 21
7	R	110/110 (100%)	107 (97%)	3 (3%)	52 43
8	H	77/77 (100%)	74 (96%)	3 (4%)	39 27
8	S	77/77 (100%)	76 (99%)	1 (1%)	76 73
9	I	47/53 (89%)	46 (98%)	1 (2%)	61 55
9	T	47/53 (89%)	45 (96%)	2 (4%)	35 23
10	J	112/112 (100%)	105 (94%)	7 (6%)	22 10
10	U	112/112 (100%)	107 (96%)	5 (4%)	34 21
11	K	93/93 (100%)	88 (95%)	5 (5%)	27 15
11	V	93/93 (100%)	90 (97%)	3 (3%)	46 35
12	W	89/88 (101%)	87 (98%)	2 (2%)	60 53
All	All	3833/3970 (96%)	3644 (95%)	189 (5%)	31 18

All (189) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	GLU
1	A	66	ASN
1	A	120	LEU
1	A	126	GLN
1	A	145	LEU
1	A	164	LEU
1	A	172	THR
1	A	179	ARG
1	A	185	LEU
1	A	188	LEU
1	A	193	LEU
1	A	239	LYS
1	A	240	LYS

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Mol	Chain	Res	Type
1	A	241	LYS
1	A	252	ARG
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	360	ASP
1	A	370	LEU
1	A	374	LEU
1	A	425	ARG
1	A	426	LEU
1	A	443	LEU
2	B	53	ARG
2	B	54	PHE
2	B	73	LEU
2	B	84	ARG
2	B	128	ARG
2	B	144	ASP
2	B	146	LEU
2	B	169	LEU
2	B	254	GLU
2	B	312	LYS
2	B	345	ASP
2	B	347	LYS
2	B	362	LEU
3	C	10	LEU
3	C	35	LEU
3	C	38	LEU
3	C	60	LEU
3	C	79	ARG
3	C	81	LEU
3	C	89	PHE
3	C	99	LYS
3	C	150	LEU
3	C	182	LEU
3	C	184	TYR
3	C	185	LEU
3	C	238	LEU
3	C	302	LEU
3	C	313	VAL

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Mol	Chain	Res	Type
3	C	336	LEU
3	C	347	PRO
3	C	350	LEU
3	C	377	LEU
3	C	382	ARG
4	D	69	LEU
4	D	113	ARG
4	D	251	VAL
4	D	256	ASN
4	D	280	LEU
4	D	283	LEU
5	E	65	LEU
5	E	114	LYS
6	F	77	GLN
6	F	89	GLU
6	F	94	LEU
6	F	130	LEU
6	F	131	GLN
7	G	16	LEU
7	G	31	GLN
7	G	91	ASN
7	G	97	GLN
7	G	127	LYS
8	H	56	PHE
8	H	60	LEU
8	H	89	LEU
9	I	55	ARG
10	J	38	ILE
10	J	39	ARG
10	J	51	TYR
10	J	59	ASN
10	J	61	ASN
10	J	68	LEU
10	J	114	GLN
11	K	30	ASN
11	K	38	GLN
11	K	81	GLU
11	K	92	ILE
11	K	93	LYS
1	L	66	ASN
1	L	76	ILE
1	L	120	LEU

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Mol	Chain	Res	Type
1	L	150	ASP
1	L	152	GLU
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	213	ASN
1	L	227	ASN
1	L	241	LYS
1	L	252	ARG
1	L	261	ILE
1	L	271	ASN
1	L	289	ASN
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	373	GLN
1	L	374	LEU
1	L	390	LEU
1	L	425	ARG
1	L	443	LEU
2	M	17	LEU
2	M	53	ARG
2	M	54	PHE
2	M	73	LEU
2	M	74	LEU
2	M	84	ARG
2	M	144	ASP
2	M	146	LEU
2	M	169	LEU
2	M	190	GLU
2	M	206	LEU
2	M	218	LYS
2	M	246	ASN
2	M	250	LEU
2	M	254	GLU

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Mol	Chain	Res	Type
2	M	292	GLN
2	M	312	LYS
2	M	330	GLU
2	M	362	LEU
3	N	35	LEU
3	N	38	LEU
3	N	79	ARG
3	N	89	PHE
3	N	99	LYS
3	N	109	PRO
3	N	150	LEU
3	N	182	LEU
3	N	184	TYR
3	N	185	LEU
3	N	208	ASN
3	N	238	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	256	ASN
4	O	280	LEU
4	O	283	LEU
5	P	41	ASP
5	P	44	LYS
5	P	45	GLU
5	P	65	LEU
5	P	211	LYS
6	Q	77	GLN
6	Q	94	LEU
6	Q	103	GLU
6	Q	111	GLN
7	R	2	PRO
7	R	16	LEU
7	R	41	LEU
8	S	87	GLU
9	T	18	VAL
9	T	55	ARG
10	U	39	ARG
10	U	51	TYR

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Mol	Chain	Res	Type
10	U	61	ASN
10	U	68	LEU
10	U	114	GLN
11	V	18	ARG
11	V	92	ILE
11	V	93	LYS
12	W	68	ASN
12	W	75	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (131) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	ASN
1	A	66	ASN
1	A	67	ASN
1	A	102	GLN
1	A	121	ASN
1	A	126	GLN
1	A	156	HIS
1	A	199	ASN
1	A	213	ASN
1	A	283	GLN
1	A	289	ASN
1	A	317	HIS
1	A	336	ASN
1	A	350	GLN
1	A	373	GLN
1	A	388	ASN
1	A	429	GLN
2	B	49	HIS
2	B	52	ASN
2	B	55	ASN
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	204	HIS
3	C	208	ASN
3	C	253	HIS
3	C	332	ASN

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Mol	Chain	Res	Type
4	D	78	HIS
4	D	79	ASN
4	D	127	ASN
5	E	38	ASN
5	E	47	ASN
5	E	106	ASN
5	E	184	HIS
6	F	77	GLN
6	F	109	GLN
6	F	110	GLN
7	G	31	GLN
7	G	53	ASN
7	G	57	GLN
7	G	79	HIS
7	G	91	ASN
7	G	97	GLN
8	H	74	ASN
9	I	14	ASN
9	I	29	GLN
10	J	59	ASN
10	J	61	ASN
10	J	77	ASN
10	J	78	GLN
10	J	114	GLN
11	K	27	GLN
11	K	30	ASN
11	K	31	ASN
11	K	34	ASN
11	K	38	GLN
11	K	89	GLN
11	K	90	HIS
11	K	91	HIS
1	L	31	GLN
1	L	47	HIS
1	L	61	ASN
1	L	66	ASN
1	L	67	ASN
1	L	102	GLN
1	L	122	GLN
1	L	127	GLN
1	L	130	ASN
1	L	136	ASN

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Mol	Chain	Res	Type
1	L	156	HIS
1	L	170	GLN
1	L	213	ASN
1	L	227	ASN
1	L	271	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	292	GLN
3	N	14	ASN
3	N	43	GLN
3	N	74	ASN
3	N	173	ASN
3	N	208	ASN
3	N	253	HIS
3	N	332	ASN
4	O	78	HIS
4	O	79	ASN
4	O	127	ASN
4	O	170	GLN
4	O	303	ASN
5	P	97	ASN
5	P	106	ASN
5	P	184	HIS
6	Q	77	GLN
6	Q	109	GLN
6	Q	119	HIS
7	R	30	ASN
7	R	53	ASN
7	R	57	GLN
7	R	79	HIS
7	R	91	ASN

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Mol	Chain	Res	Type
8	S	55	GLN
8	S	74	ASN
9	T	14	ASN
9	T	29	GLN
10	U	61	ASN
10	U	77	ASN
10	U	78	GLN
10	U	114	GLN
11	V	31	ASN
11	V	34	ASN
11	V	38	GLN
11	V	89	GLN
11	V	90	HIS
11	V	91	HIS
12	W	67	ASN
12	W	68	ASN
12	W	75	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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	77	12	10,11,12	0.88	0	12,14,16	1.04	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	77	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	77	M3L	CM2-NZ-CM1	-2.07	103.64	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)

25 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	6PH	A	4013	-	39,39,39	0.98	2 (5%)	42,44,44	1.29	4 (9%)
15	UMQ	A	4021	-	35,35,35	0.90	1 (2%)	46,46,46	1.78	7 (15%)
16	HEM	C	4001	3	30,50,50	3.07	11 (36%)	24,82,82	2.41	9 (37%)
16	HEM	C	4002	3	30,50,50	2.87	11 (36%)	24,82,82	2.57	7 (29%)
17	SMA	C	4005	-	35,38,38	1.28	3 (8%)	40,52,52	1.49	4 (10%)
18	8PE	C	4010	-	45,46,46	0.93	2 (4%)	46,51,51	1.19	3 (6%)
19	9PE	C	4011	-	38,39,39	0.65	0	39,44,44	0.96	1 (2%)
20	CN5	C	4033	-	40,40,40	1.56	7 (17%)	42,48,48	1.70	7 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
16	HEM	D	4003	4	30,50,50	2.68	8 (26%)	24,82,82	3.06	8 (33%)
21	7PH	D	4014	-	37,37,37	0.97	1 (2%)	40,42,42	1.46	9 (22%)
22	CN3	D	4031	-	54,54,54	1.47	10 (18%)	56,66,66	1.43	5 (8%)
23	FES	E	4004	5	0,4,4	0.00	-	0,4,4	0.00	-
14	6PH	L	4113	-	39,39,39	0.99	2 (5%)	42,44,44	1.32	4 (9%)
15	UMQ	L	4121	-	35,35,35	0.93	1 (2%)	46,46,46	1.74	6 (13%)
16	HEM	N	4021	3	30,50,50	3.03	11 (36%)	24,82,82	2.07	8 (33%)
16	HEM	N	4022	3	30,50,50	2.91	12 (40%)	24,82,82	2.42	8 (33%)
17	SMA	N	4025	-	35,38,38	1.24	3 (8%)	40,52,52	1.57	5 (12%)
18	8PE	N	4110	-	45,46,46	0.97	4 (8%)	46,51,51	1.15	2 (4%)
19	9PE	N	4111	-	38,39,39	0.69	0	39,44,44	0.99	1 (2%)
22	CN3	N	4131	-	54,54,54	1.45	10 (18%)	56,66,66	1.41	5 (8%)
16	HEM	O	4023	4	30,50,50	2.63	9 (30%)	24,82,82	3.30	8 (33%)
21	7PH	O	4114	-	37,37,37	0.97	2 (5%)	40,42,42	1.46	9 (22%)
13	SUC	O	4146	-	24,24,24	0.52	0	36,36,36	0.67	1 (2%)
23	FES	P	4024	5	0,4,4	0.00	-	0,4,4	0.00	-
16	HEM	W	4026	12	30,50,50	2.57	8 (26%)	24,82,82	2.96	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	6PH	A	4013	-	-	0/41/41/41	0/0/0/0
15	UMQ	A	4021	-	-	0/20/60/60	0/2/2/2
16	HEM	C	4001	3	-	0/10/54/54	0/0/8/8
16	HEM	C	4002	3	-	0/10/54/54	0/0/8/8
17	SMA	C	4005	-	-	0/33/34/34	0/2/2/2
18	8PE	C	4010	-	-	0/50/50/50	0/0/0/0
19	9PE	C	4011	-	-	0/43/43/43	0/0/0/0
20	CN5	C	4033	-	-	0/44/44/44	0/0/0/0
16	HEM	D	4003	4	-	0/10/54/54	0/0/8/8
21	7PH	D	4014	-	-	0/39/39/39	0/0/0/0
22	CN3	D	4031	-	-	0/65/65/65	0/0/0/0
23	FES	E	4004	5	-	0/0/4/4	0/1/1/1
14	6PH	L	4113	-	-	0/41/41/41	0/0/0/0
15	UMQ	L	4121	-	-	0/20/60/60	0/2/2/2
16	HEM	N	4021	3	-	0/10/54/54	0/0/8/8

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	HEM	N	4022	3	-	0/10/54/54	0/0/8/8
17	SMA	N	4025	-	-	0/33/34/34	0/2/2/2
18	8PE	N	4110	-	-	0/50/50/50	0/0/0/0
19	9PE	N	4111	-	-	0/43/43/43	0/0/0/0
22	CN3	N	4131	-	-	0/65/65/65	0/0/0/0
16	HEM	O	4023	4	-	0/10/54/54	0/0/8/8
21	7PH	O	4114	-	-	0/39/39/39	0/0/0/0
13	SUC	O	4146	-	-	0/12/51/51	0/2/2/2
23	FES	P	4024	5	-	0/0/4/4	0/1/1/1
16	HEM	W	4026	12	-	0/10/54/54	0/0/8/8

All (118) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	C	4001	HEM	C3B-C4B	-8.91	1.43	1.51
16	D	4003	HEM	C3B-C4B	-7.97	1.44	1.51
16	N	4021	HEM	C3B-C4B	-7.91	1.44	1.51
16	N	4022	HEM	C3B-C4B	-7.79	1.44	1.51
16	W	4026	HEM	C3B-C4B	-7.51	1.45	1.51
16	C	4002	HEM	C3B-C4B	-7.22	1.45	1.51
16	O	4023	HEM	C3B-C4B	-7.17	1.45	1.51
16	C	4001	HEM	C3C-CAC	-6.36	1.39	1.51
16	C	4002	HEM	C2D-C3D	-6.32	1.35	1.54
16	N	4021	HEM	C3C-CAC	-6.32	1.39	1.51
16	N	4022	HEM	C2D-C3D	-6.31	1.35	1.54
16	N	4021	HEM	C2D-C3D	-6.27	1.35	1.54
16	C	4001	HEM	C2D-C3D	-6.19	1.35	1.54
16	D	4003	HEM	C2D-C3D	-6.18	1.36	1.54
16	O	4023	HEM	C2D-C3D	-6.16	1.36	1.54
16	W	4026	HEM	C2D-C3D	-6.04	1.36	1.54
16	N	4022	HEM	C3D-C4D	-5.99	1.43	1.51
16	C	4002	HEM	C3D-C4D	-5.97	1.43	1.51
16	N	4021	HEM	C3B-CAB	-5.95	1.40	1.51
16	C	4001	HEM	C3B-CAB	-5.94	1.40	1.51
16	N	4021	HEM	C3D-C4D	-5.76	1.44	1.51
16	D	4003	HEM	C3D-C4D	-5.60	1.44	1.51
16	N	4022	HEM	C3B-CAB	-5.46	1.41	1.51
16	C	4001	HEM	C3D-C4D	-5.45	1.44	1.51
16	O	4023	HEM	C3D-C4D	-5.23	1.44	1.51
16	N	4022	HEM	C3C-CAC	-5.09	1.41	1.51
16	C	4002	HEM	C3B-CAB	-5.03	1.41	1.51
16	W	4026	HEM	C3D-C4D	-4.99	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	C	4002	HEM	C3C-CAC	-4.93	1.42	1.51
16	O	4023	HEM	C2C-C1C	-4.49	1.44	1.52
22	D	4031	CN3	O31-C3	-4.37	1.35	1.45
22	N	4131	CN3	O31-C3	-4.36	1.35	1.45
16	C	4001	HEM	C2C-C1C	-4.27	1.44	1.52
16	N	4021	HEM	C2C-C1C	-4.23	1.44	1.52
16	D	4003	HEM	C2C-C1C	-4.22	1.44	1.52
16	N	4022	HEM	C2C-C1C	-4.00	1.45	1.52
16	W	4026	HEM	C2C-C1C	-3.98	1.45	1.52
16	C	4002	HEM	C2C-C1C	-3.88	1.45	1.52
21	D	4014	7PH	O31-C3	-3.59	1.37	1.45
21	O	4114	7PH	O31-C3	-3.48	1.37	1.45
22	D	4031	CN3	O21-C2	-3.43	1.37	1.46
22	D	4031	CN3	O3'-CA	-3.36	1.31	1.44
15	A	4021	UMQ	C3-C2	-3.36	1.43	1.52
15	L	4121	UMQ	C3-C2	-3.35	1.43	1.52
22	N	4131	CN3	O3'-CA	-3.29	1.31	1.44
22	N	4131	CN3	O21-C2	-3.29	1.38	1.46
20	C	4033	CN5	O3'-CA	-3.23	1.31	1.44
22	N	4131	CN3	O32-C31	-2.79	1.14	1.22
16	C	4002	HEM	C2D-C1D	-2.57	1.43	1.51
22	D	4031	CN3	O32-C31	-2.56	1.15	1.22
22	D	4031	CN3	O11-C1	-2.49	1.34	1.44
18	N	4110	8PE	O32-C31	-2.36	1.15	1.22
22	N	4131	CN3	O11-C1	-2.33	1.35	1.44
16	C	4002	HEM	C2B-C1B	-2.26	1.44	1.51
22	N	4131	CN3	O41-C3'	-2.25	1.40	1.45
18	C	4010	8PE	O32-C31	-2.25	1.15	1.22
16	W	4026	HEM	C2B-C1B	-2.24	1.44	1.51
16	C	4001	HEM	C2D-C1D	-2.23	1.44	1.51
16	N	4022	HEM	C2D-C1D	-2.22	1.44	1.51
16	N	4021	HEM	C2D-C1D	-2.20	1.44	1.51
16	C	4001	HEM	C2B-C1B	-2.20	1.44	1.51
16	D	4003	HEM	C2B-C1B	-2.19	1.44	1.51
16	O	4023	HEM	C2B-C1B	-2.18	1.44	1.51
16	N	4021	HEM	C2B-C1B	-2.17	1.44	1.51
16	N	4022	HEM	C2B-C1B	-2.17	1.44	1.51
16	D	4003	HEM	C2D-C1D	-2.13	1.44	1.51
22	D	4031	CN3	C1-C2	-2.11	1.44	1.50
16	W	4026	HEM	C2D-C1D	-2.07	1.45	1.51
16	O	4023	HEM	C2D-C1D	-2.04	1.45	1.51
21	O	4114	7PH	O22-C21	-2.04	1.16	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	N	4022	HEM	C1C-NC	2.03	1.38	1.36
16	N	4021	HEM	FE-NC	2.07	2.04	1.95
22	D	4031	CN3	CA-CB	2.07	1.59	1.51
22	N	4131	CN3	OA-CB	2.13	1.49	1.43
22	N	4131	CN3	CC-CB	2.13	1.59	1.51
22	N	4131	CN3	CA-CB	2.16	1.59	1.51
18	N	4110	8PE	C3-C2	2.16	1.56	1.50
16	C	4001	HEM	FE-NC	2.18	2.04	1.95
16	N	4022	HEM	CMA-C3A	2.18	1.56	1.51
16	O	4023	HEM	FE-NC	2.19	2.04	1.95
22	D	4031	CN3	CC-CB	2.19	1.60	1.51
22	D	4031	CN3	OA-CB	2.21	1.50	1.43
16	C	4001	HEM	CBB-CAB	2.24	1.42	1.29
17	C	4005	SMA	C4-C3	2.26	1.47	1.41
20	C	4033	CN5	CC-CB	2.27	1.60	1.51
20	C	4033	CN5	P'-O4'	2.31	1.64	1.54
22	D	4031	CN3	O21-C21	2.37	1.41	1.34
18	N	4110	8PE	C1-C2	2.38	1.57	1.50
17	N	4025	SMA	C4-C3	2.40	1.48	1.41
22	N	4131	CN3	O21-C21	2.41	1.41	1.34
14	A	4013	6PH	C3-C2	2.43	1.57	1.50
16	N	4021	HEM	CBC-CAC	2.44	1.43	1.29
16	N	4022	HEM	CBC-CAC	2.46	1.43	1.29
16	C	4001	HEM	CBC-CAC	2.48	1.43	1.29
14	A	4013	6PH	C1-C2	2.51	1.57	1.50
16	C	4002	HEM	CMA-C3A	2.52	1.56	1.51
16	N	4021	HEM	CBB-CAB	2.53	1.43	1.29
20	C	4033	CN5	P-O11	2.56	1.70	1.59
14	L	4113	6PH	C3-C2	2.59	1.58	1.50
16	C	4002	HEM	CBC-CAC	2.66	1.44	1.29
14	L	4113	6PH	C1-C2	2.68	1.58	1.50
20	C	4033	CN5	OA-CB	2.76	1.51	1.43
16	N	4022	HEM	CBB-CAB	2.80	1.45	1.29
17	C	4005	SMA	O1-C2	2.82	1.38	1.35
20	C	4033	CN5	P'-O2'	2.86	1.61	1.51
18	N	4110	8PE	O21-C21	3.13	1.43	1.34
17	N	4025	SMA	O1-C2	3.15	1.38	1.35
18	C	4010	8PE	O21-C21	3.22	1.43	1.34
16	C	4002	HEM	CBB-CAB	3.28	1.48	1.29
20	C	4033	CN5	P-O14	3.52	1.64	1.51
16	W	4026	HEM	CBB-CAB	4.08	1.52	1.29
16	D	4003	HEM	CBB-CAB	4.19	1.53	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	W	4026	HEM	CBC-CAC	4.21	1.53	1.29
16	O	4023	HEM	CBB-CAB	4.27	1.54	1.29
16	O	4023	HEM	CBC-CAC	4.35	1.54	1.29
16	D	4003	HEM	CBC-CAC	4.35	1.54	1.29
17	N	4025	SMA	C4-C4A	5.18	1.48	1.41
17	C	4005	SMA	C4-C4A	5.42	1.48	1.41

All (130) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	O	4023	HEM	C3B-CAB-CBB	-9.05	110.57	124.46
15	A	4021	UMQ	CA-O1'-C1'	-8.58	98.95	113.94
15	L	4121	UMQ	CA-O1'-C1'	-8.30	99.44	113.94
16	O	4023	HEM	C3C-CAC-CBC	-8.18	111.90	124.46
16	D	4003	HEM	C3C-CAC-CBC	-8.07	112.07	124.46
16	W	4026	HEM	C3B-CAB-CBB	-7.65	112.73	124.46
16	D	4003	HEM	C3B-CAB-CBB	-7.47	112.99	124.46
16	W	4026	HEM	C3C-CAC-CBC	-6.76	114.09	124.46
22	D	4031	CN3	C2'-O51-C51	-5.36	105.03	117.89
16	C	4001	HEM	C3C-CAC-CBC	-5.14	116.57	124.46
22	N	4131	CN3	C2'-O51-C51	-5.12	105.60	117.89
17	C	4005	SMA	C3-C4-C4A	-4.87	114.60	121.35
17	N	4025	SMA	C3-C4-C4A	-4.74	114.77	121.35
20	C	4033	CN5	C3'-C2'-C1'	-4.52	97.68	113.85
17	N	4025	SMA	C9-C10-C11	-4.36	109.61	114.75
14	L	4113	6PH	C3-C2-C1	-4.17	102.31	112.07
14	A	4013	6PH	C3-C2-C1	-4.15	102.36	112.07
19	N	4111	9PE	C2-O21-C21	-3.93	108.47	117.89
22	N	4131	CN3	C2-O21-C21	-3.92	108.50	117.89
22	D	4031	CN3	C2-O21-C21	-3.75	108.89	117.89
22	D	4031	CN3	C3-C2-C1	-3.69	103.44	112.07
19	C	4011	9PE	C2-O21-C21	-3.69	109.04	117.89
17	C	4005	SMA	C9-C10-C11	-3.69	110.41	114.75
20	C	4033	CN5	P'-O1'-C1'	-3.59	100.98	121.50
18	C	4010	8PE	C2-O21-C21	-3.59	109.29	117.89
21	D	4014	7PH	C38-C37-C36	-3.58	96.04	114.53
20	C	4033	CN5	O11-C1-C2	-3.56	95.52	108.85
22	N	4131	CN3	C3-C2-C1	-3.55	103.77	112.07
21	O	4114	7PH	C38-C37-C36	-3.54	96.23	114.53
18	N	4110	8PE	C2-O21-C21	-3.48	109.54	117.89
21	D	4014	7PH	C3-C2-C1	-3.13	104.74	112.07
22	D	4031	CN3	C3'-C2'-C1'	-3.13	104.75	112.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	O	4114	7PH	C3-C2-C1	-3.01	105.03	112.07
16	N	4022	HEM	CAA-C2A-C1A	-2.94	123.82	127.01
21	D	4014	7PH	O11-P-O14	-2.90	99.76	107.14
16	C	4001	HEM	CAA-C2A-C1A	-2.83	123.93	127.01
21	O	4114	7PH	O11-P-O14	-2.75	100.14	107.14
16	N	4021	HEM	CBA-CAA-C2A	-2.66	107.77	112.53
13	O	4146	SUC	C4-C3-C2	-2.61	105.92	110.79
22	N	4131	CN3	C3'-C2'-C1'	-2.59	106.02	112.07
21	O	4114	7PH	O31-C3-C2	-2.56	101.79	108.69
15	A	4021	UMQ	O1-C1-O5	-2.53	104.27	110.68
15	A	4021	UMQ	CD-CC-CB	-2.47	101.79	114.53
15	L	4121	UMQ	C3'-C4'-C5'	-2.42	105.37	110.84
15	L	4121	UMQ	CD-CC-CB	-2.37	102.29	114.53
21	D	4014	7PH	O31-C3-C2	-2.37	102.32	108.69
14	L	4113	6PH	O14-P-O11	-2.36	99.78	106.56
15	A	4021	UMQ	C3'-C4'-C5'	-2.32	105.59	110.84
21	O	4114	7PH	O31-C31-C32	-2.32	104.84	111.90
16	N	4021	HEM	C3C-CAC-CBC	-2.28	120.96	124.46
20	C	4033	CN5	C3-C2-C1	-2.26	105.76	113.85
21	D	4014	7PH	O31-C31-C32	-2.25	105.04	111.90
16	W	4026	HEM	CBA-CAA-C2A	-2.24	108.52	112.53
21	O	4114	7PH	O12-P-O14	-2.23	103.39	110.58
21	D	4014	7PH	O12-P-O14	-2.22	103.43	110.58
14	A	4013	6PH	O14-P-O11	-2.18	100.29	106.56
15	L	4121	UMQ	O1-C1-O5	-2.17	105.19	110.68
20	C	4033	CN5	C3-O31-C31	-2.11	111.12	117.02
15	A	4021	UMQ	C1-O5-C5	-2.06	109.74	113.75
18	C	4010	8PE	O31-C3-C2	-2.01	103.27	108.69
22	D	4031	CN3	O4'-P'-O3'	2.05	118.79	108.46
17	C	4005	SMA	C4-C3-C2	2.12	120.81	117.73
17	N	4025	SMA	C4-C3-C2	2.14	120.84	117.73
17	N	4025	SMA	O8-C8-C7	2.15	124.07	119.34
21	D	4014	7PH	O31-C31-O32	2.19	129.15	123.49
21	O	4114	7PH	O31-C31-O32	2.19	129.15	123.49
22	N	4131	CN3	O4'-P'-O3'	2.23	119.69	108.46
20	C	4033	CN5	C33-C32-C31	2.29	122.59	113.59
16	N	4022	HEM	CMD-C2D-C3D	2.45	125.18	114.35
16	C	4001	HEM	CMD-C2D-C3D	2.51	125.44	114.35
16	C	4002	HEM	CMD-C2D-C3D	2.66	126.12	114.35
21	O	4114	7PH	O13-P-O11	2.71	114.36	106.56
21	D	4014	7PH	O13-P-O11	2.73	114.42	106.56
16	N	4021	HEM	CMD-C2D-C3D	2.78	126.63	114.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	4013	6PH	O13-P-O11	2.81	114.67	106.56
15	A	4021	UMQ	O1'-C1'-C2'	2.83	111.61	108.04
16	C	4001	HEM	C3B-CAB-CBB	2.90	128.91	124.46
15	L	4121	UMQ	O1'-C1'-C2'	2.91	111.71	108.04
16	D	4003	HEM	CMD-C2D-C3D	2.91	127.24	114.35
16	W	4026	HEM	CMD-C2D-C3D	2.94	127.34	114.35
14	L	4113	6PH	O13-P-O11	2.96	115.10	106.56
15	A	4021	UMQ	O1'-CA-CB	3.02	121.89	109.88
18	N	4110	8PE	C3-C2-C1	3.02	119.14	112.07
16	O	4023	HEM	CMD-C2D-C3D	3.10	128.05	114.35
16	N	4022	HEM	C2D-C3D-C4D	3.13	106.80	101.50
21	D	4014	7PH	O12-P-O11	3.16	115.68	106.56
21	O	4114	7PH	O12-P-O11	3.19	115.75	106.56
16	W	4026	HEM	C2D-C3D-C4D	3.22	106.96	101.50
15	L	4121	UMQ	O1'-CA-CB	3.22	122.69	109.88
16	D	4003	HEM	C2D-C3D-C4D	3.22	106.97	101.50
16	C	4002	HEM	C2D-C3D-C4D	3.27	107.04	101.50
16	N	4021	HEM	C2D-C3D-C4D	3.29	107.08	101.50
16	O	4023	HEM	C2D-C3D-C4D	3.29	107.08	101.50
16	C	4001	HEM	C2D-C3D-C4D	3.34	107.15	101.50
18	C	4010	8PE	C3-C2-C1	3.38	119.99	112.07
14	L	4113	6PH	O11-P-O12	3.44	115.89	107.14
14	A	4013	6PH	O11-P-O12	3.48	116.01	107.14
16	N	4021	HEM	CMC-C2C-C3C	3.50	125.26	116.53
16	C	4001	HEM	CMC-C2C-C3C	3.52	125.32	116.53
16	N	4021	HEM	CMB-C2B-C3B	3.55	125.40	116.53
16	N	4022	HEM	C3B-CAB-CBB	3.56	129.91	124.46
16	O	4023	HEM	CAD-C3D-C4D	3.60	125.15	112.47
16	N	4021	HEM	CAD-C3D-C2D	3.62	123.63	113.22
16	C	4001	HEM	CAD-C3D-C2D	3.73	123.94	113.22
16	D	4003	HEM	CAD-C3D-C4D	3.79	125.84	112.47
16	W	4026	HEM	CAD-C3D-C2D	3.96	124.59	113.22
16	C	4002	HEM	CAD-C3D-C4D	4.06	126.80	112.47
16	W	4026	HEM	CMB-C2B-C3B	4.14	126.87	116.53
16	W	4026	HEM	CMC-C2C-C3C	4.15	126.89	116.53
16	N	4022	HEM	CAD-C3D-C4D	4.29	127.59	112.47
16	N	4022	HEM	CAD-C3D-C2D	4.31	125.61	113.22
16	D	4003	HEM	CMC-C2C-C3C	4.40	127.52	116.53
16	D	4003	HEM	CMB-C2B-C3B	4.45	127.64	116.53
16	C	4002	HEM	CAD-C3D-C2D	4.50	126.16	113.22
16	W	4026	HEM	CAD-C3D-C4D	4.50	128.36	112.47
16	O	4023	HEM	CMB-C2B-C3B	4.58	127.97	116.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	O	4023	HEM	CMC-C2C-C3C	4.65	128.13	116.53
16	C	4001	HEM	CAD-C3D-C4D	4.66	128.91	112.47
16	N	4021	HEM	CAD-C3D-C4D	4.74	129.19	112.47
17	C	4005	SMA	C9-C2-C3	4.75	126.83	120.56
16	C	4001	HEM	CMB-C2B-C3B	4.77	128.43	116.53
16	D	4003	HEM	CAD-C3D-C2D	4.86	127.19	113.22
16	N	4022	HEM	CMB-C2B-C3B	5.01	129.04	116.53
16	O	4023	HEM	CAD-C3D-C2D	5.04	127.72	113.22
16	C	4002	HEM	CMB-C2B-C3B	5.18	129.45	116.53
17	N	4025	SMA	C9-C2-C3	5.37	127.65	120.56
16	C	4002	HEM	C3B-CAB-CBB	5.60	133.04	124.46
20	C	4033	CN5	O1'-C1'-C2'	5.73	130.30	108.85
16	N	4022	HEM	CMC-C2C-C3C	5.94	131.36	116.53
16	C	4002	HEM	CMC-C2C-C3C	5.98	131.46	116.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

17 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	4013	6PH	1	0
15	A	4021	UMQ	2	0
16	C	4001	HEM	1	0
16	C	4002	HEM	1	0
17	C	4005	SMA	1	0
18	C	4010	8PE	1	0
20	C	4033	CN5	5	0
16	D	4003	HEM	1	0
21	D	4014	7PH	2	0
22	D	4031	CN3	5	0
14	L	4113	6PH	3	0
15	L	4121	UMQ	2	0
16	N	4021	HEM	2	0
16	N	4022	HEM	1	0
22	N	4131	CN3	5	0
21	O	4114	7PH	2	0
13	O	4146	SUC	5	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%)	0.57	50 (11%) 6 7	26, 44, 98, 114	0
1	L	431/431 (100%)	0.50	42 (9%) 10 11	25, 42, 90, 113	0
2	B	352/352 (100%)	0.63	34 (9%) 10 11	30, 47, 73, 114	0
2	M	352/352 (100%)	0.58	36 (10%) 9 10	32, 45, 72, 109	0
3	C	385/385 (100%)	-0.14	4 (1%) 84 86	18, 27, 38, 91	0
3	N	385/385 (100%)	-0.19	4 (1%) 84 86	19, 26, 37, 88	0
4	D	248/248 (100%)	0.03	11 (4%) 38 41	25, 35, 57, 83	0
4	O	248/248 (100%)	-0.02	7 (2%) 56 60	24, 33, 55, 86	0
5	E	185/185 (100%)	0.49	15 (8%) 15 16	24, 40, 69, 94	0
5	P	185/185 (100%)	0.69	24 (12%) 5 5	24, 41, 80, 93	0
6	F	74/146 (50%)	0.86	12 (16%) 3 3	34, 46, 90, 96	0
6	Q	74/146 (50%)	0.80	13 (17%) 2 2	32, 45, 87, 90	0
7	G	126/126 (100%)	-0.01	7 (5%) 28 31	26, 37, 60, 78	0
7	R	126/126 (100%)	0.01	6 (4%) 34 37	23, 34, 62, 80	0
8	H	93/93 (100%)	1.90	27 (29%) 1 0	24, 45, 128, 131	0
8	S	93/93 (100%)	1.33	21 (22%) 1 1	22, 43, 113, 119	0
9	I	57/65 (87%)	0.87	7 (12%) 5 6	34, 42, 83, 100	0
9	T	57/65 (87%)	0.80	8 (14%) 4 4	32, 40, 84, 96	0
10	J	127/127 (100%)	0.97	21 (16%) 2 2	40, 57, 71, 80	0
10	U	127/127 (100%)	1.16	24 (18%) 2 2	42, 59, 73, 82	0
11	K	107/107 (100%)	2.32	51 (47%) 0 0	51, 81, 114, 116	0
11	V	107/107 (100%)	2.87	67 (62%) 0 0	60, 92, 120, 122	0
12	W	107/108 (99%)	1.47	27 (25%) 1 1	46, 62, 87, 99	0
All	All	4477/4638 (96%)	0.55	518 (11%) 6 7	18, 41, 90, 131	0

All (518) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
8	H	46	PHE	20.0
2	B	338	LEU	19.0
1	L	230	LEU	18.1
9	I	57	ALA	14.0
9	T	58	ALA	13.7
1	A	27	ALA	12.9
8	H	42	HIS	12.0
1	A	228	LEU	11.4
8	H	45	VAL	11.2
8	H	49	PHE	11.2
9	I	58	ALA	11.1
8	S	49	PHE	10.7
12	W	1	THR	10.4
1	A	230	LEU	10.3
2	B	332	VAL	10.1
8	S	46	PHE	9.8
8	H	41	PHE	9.7
11	V	15	LEU	9.6
2	B	336	ILE	9.6
8	S	40	ILE	9.4
9	T	57	ALA	9.4
3	C	384	ASN	9.2
1	A	129	ALA	9.1
11	V	106	ILE	9.0
3	N	384	ASN	9.0
8	H	44	ALA	9.0
1	L	27	ALA	8.9
2	M	338	LEU	8.5
11	V	79	GLU	8.4
11	V	29	ILE	8.3
8	S	94	VAL	8.1
11	K	106	ILE	8.1
2	M	336	ILE	8.0
6	Q	119	HIS	7.9
8	H	39	GLY	7.8
8	S	41	PHE	7.8
8	H	94	VAL	7.8
1	A	128	LYS	7.7
8	H	52	PHE	7.7
1	L	227	ASN	7.6
8	H	40	ILE	7.5
3	C	383	VAL	7.5

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Mol	Chain	Res	Type	RSRZ
6	F	119	HIS	7.4
8	H	43	ASN	7.4
2	M	330	GLU	7.4
5	E	47	ASN	7.4
8	H	37	LEU	7.4
11	K	11	LEU	7.3
11	K	9	VAL	7.3
1	L	229	SER	7.3
8	H	51	ARG	7.3
11	V	14	SER	7.2
8	H	47	ASN	7.2
8	S	38	GLN	7.2
9	I	2	SER	7.0
1	A	234	THR	6.9
4	O	308	ARG	6.9
8	S	42	HIS	6.9
3	N	385	LYS	6.9
8	S	39	GLY	6.8
11	K	107	LYS	6.8
1	A	232	THR	6.8
5	E	46	ASN	6.7
1	A	231	GLN	6.7
1	A	215	LYS	6.6
3	C	385	LYS	6.6
11	K	80	PRO	6.6
11	K	79	GLU	6.5
4	D	308	ARG	6.5
2	M	332	VAL	6.5
5	P	46	ASN	6.5
5	P	100	ALA	6.4
8	S	44	ALA	6.3
12	W	9	LYS	6.3
11	V	80	PRO	6.3
11	K	42	GLY	6.2
11	V	107	LYS	6.2
6	Q	118	GLU	6.1
6	F	115	ALA	5.9
6	F	117	LEU	5.9
4	O	309	LYS	5.9
11	V	24	ARG	5.9
8	S	37	LEU	5.9
1	A	229	SER	5.9

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Mol	Chain	Res	Type	RSRZ
11	K	16	GLY	5.9
1	A	227	ASN	5.8
7	R	127	LYS	5.7
8	H	38	GLN	5.6
8	H	48	SER	5.6
5	P	45	GLU	5.5
2	B	211	ALA	5.4
6	F	118	GLU	5.4
5	E	103	LEU	5.4
10	U	45	LYS	5.4
5	P	47	ASN	5.3
5	P	213	ILE	5.3
10	U	55	VAL	5.2
11	V	65	SER	5.2
12	W	55	ASP	5.2
11	K	75	ILE	5.2
1	L	234	THR	5.1
3	N	383	VAL	5.1
5	P	211	LYS	5.1
1	L	28	GLU	5.1
10	U	66	ASP	5.1
11	V	70	ASP	5.0
1	L	125	ILE	5.0
11	K	14	SER	5.0
8	S	52	PHE	4.9
1	A	381	GLY	4.9
1	L	231	GLN	4.9
2	B	337	GLU	4.9
10	J	42	PRO	4.9
2	M	333	SER	4.9
1	L	29	VAL	4.9
11	K	24	ARG	4.8
1	A	130	ASN	4.8
9	T	55	ARG	4.8
5	E	49	ALA	4.8
2	M	344	LYS	4.8
11	V	103	LYS	4.7
11	V	83	ILE	4.7
11	V	100	ALA	4.7
10	U	65	LYS	4.7
9	I	56	ILE	4.7
10	U	43	GLY	4.7

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Mol	Chain	Res	Type	RSRZ
4	D	210	PRO	4.7
11	K	43	THR	4.6
4	D	309	LYS	4.6
5	E	210	ASP	4.6
6	F	116	ASP	4.6
7	G	127	LYS	4.6
11	V	33	LEU	4.6
1	A	44	PRO	4.6
2	M	329	ASN	4.6
11	K	40	PRO	4.6
1	A	28	GLU	4.5
12	W	108	GLU	4.5
10	J	45	LYS	4.5
1	L	129	ALA	4.5
2	B	218	LYS	4.5
11	V	4	LEU	4.5
10	U	42	PRO	4.5
11	V	3	GLU	4.4
1	L	238	LEU	4.4
8	S	43	ASN	4.4
5	E	45	GLU	4.4
6	Q	116	ASP	4.4
1	L	128	LYS	4.4
11	V	7	THR	4.4
5	P	91	MET	4.4
11	K	10	SER	4.3
4	O	210	PRO	4.3
11	V	18	ARG	4.3
9	T	2	SER	4.3
2	M	339	ASN	4.3
1	A	127	GLN	4.2
8	S	45	VAL	4.2
2	M	211	ALA	4.2
11	V	11	LEU	4.2
11	K	70	ASP	4.2
1	A	271	ASN	4.2
6	F	112	PRO	4.1
5	E	153	LEU	4.1
5	P	153	LEU	4.1
11	V	75	ILE	4.1
12	W	107	CYS	4.1
6	Q	112	PRO	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	225	SER	4.1
12	W	28	GLY	4.1
11	V	88	CYS	4.1
11	K	17	ASP	4.1
6	Q	115	ALA	4.1
8	H	53	LYS	4.1
11	V	60	SER	4.0
11	V	35	TRP	4.0
2	B	331	SER	4.0
10	U	127	PRO	4.0
1	L	217	GLU	4.0
2	M	218	LYS	4.0
3	N	156	PHE	4.0
2	M	341	ASP	4.0
11	V	105	GLU	3.9
11	V	86	TYR	3.9
11	K	65	SER	3.9
10	J	127	PRO	3.9
1	L	457	TRP	3.9
11	V	9	VAL	3.9
1	L	225	SER	3.9
12	W	94	LYS	3.9
1	L	130	ASN	3.9
12	W	49	GLU	3.9
5	P	210	ASP	3.9
2	M	166	ARG	3.8
11	K	15	LEU	3.8
10	U	83	LEU	3.7
1	A	35	GLY	3.7
1	A	30	THR	3.7
1	L	233	GLY	3.7
11	V	41	ASP	3.7
11	K	29	ILE	3.7
1	A	29	VAL	3.7
12	W	50	GLY	3.7
1	L	44	PRO	3.7
5	P	49	ALA	3.7
2	M	318	ILE	3.7
12	W	27	LYS	3.7
8	H	4	PRO	3.6
10	J	65	LYS	3.6
11	V	17	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
1	L	32	LEU	3.6
11	V	8	PRO	3.6
10	U	15	SER	3.6
1	A	32	LEU	3.6
2	B	22	ARG	3.6
12	W	42	GLY	3.6
11	K	23	CYS	3.6
11	K	41	ASP	3.6
11	V	28	ASP	3.6
11	K	86	TYR	3.5
1	L	232	THR	3.5
11	K	7	THR	3.5
11	V	30	ASN	3.5
6	F	74	VAL	3.5
1	L	31	GLN	3.5
4	D	211	GLY	3.5
10	U	44	ASN	3.5
5	E	100	ALA	3.5
1	L	35	GLY	3.5
2	B	266	GLU	3.5
11	V	12	ALA	3.5
8	S	86	ARG	3.5
1	L	271	ASN	3.5
1	L	235	LYS	3.5
11	V	10	SER	3.5
1	A	125	ILE	3.5
1	L	215	LYS	3.5
1	A	126	GLN	3.4
9	T	26	PHE	3.4
11	V	69	THR	3.4
5	P	208	ASP	3.4
10	U	31	SER	3.4
1	A	124	PHE	3.4
5	E	89	LEU	3.4
11	V	34	ASN	3.4
1	L	126	GLN	3.4
2	B	330	GLU	3.4
11	K	104	LEU	3.4
1	A	457	TRP	3.4
11	V	23	CYS	3.4
7	G	23	LYS	3.4
1	A	31	GLN	3.3

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Mol	Chain	Res	Type	RSRZ
11	K	100	ALA	3.3
11	K	73	LEU	3.3
11	K	74	THR	3.3
10	J	43	GLY	3.3
2	B	339	ASN	3.3
11	V	43	THR	3.3
3	C	156	PHE	3.2
8	H	68	TYR	3.2
1	L	239	LYS	3.2
8	S	2	GLY	3.2
2	B	166	ARG	3.2
1	A	45	SER	3.2
12	W	4	LYS	3.2
5	P	48	ASP	3.2
5	E	91	MET	3.2
11	V	32	PHE	3.2
2	B	213	LYS	3.2
2	B	333	SER	3.2
2	B	17	LEU	3.2
10	U	62	PRO	3.2
1	A	241	LYS	3.1
11	V	13	ALA	3.1
11	V	104	LEU	3.1
11	K	94	PHE	3.1
11	V	36	TYR	3.1
11	K	103	LYS	3.1
12	W	26	GLU	3.1
2	B	368	LEU	3.1
11	K	88	CYS	3.1
2	M	238	VAL	3.1
10	J	62	PRO	3.1
11	K	81	GLU	3.1
5	P	97	ASN	3.1
10	J	76	LYS	3.1
11	V	39	LYS	3.1
2	M	50	LEU	3.0
11	V	20	THR	3.0
1	A	219	LEU	3.0
2	M	250	LEU	3.0
11	V	81	GLU	3.0
1	A	233	GLY	3.0
10	J	125	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
11	K	87	PHE	3.0
12	W	59	LYS	3.0
1	L	208	VAL	3.0
1	L	240	LYS	3.0
11	V	73	LEU	3.0
8	H	56	PHE	2.9
9	T	3	PHE	2.9
11	V	94	PHE	2.9
10	U	81	LEU	2.9
1	L	236	PRO	2.9
7	R	20	VAL	2.9
8	H	7	LYS	2.9
12	W	21[A]	GLN	2.9
2	B	347	LYS	2.9
6	F	106	LYS	2.9
8	S	5	SER	2.9
4	D	286	TRP	2.9
12	W	5	ALA	2.9
12	W	92	LYS	2.9
11	V	59	PRO	2.8
11	K	3	GLU	2.8
11	V	21	ILE	2.8
1	A	240	LYS	2.8
2	B	50	LEU	2.8
7	R	23	LYS	2.8
11	K	60	SER	2.8
11	K	77	ASN	2.8
2	M	266	GLU	2.8
11	V	74	THR	2.8
2	B	238	VAL	2.8
11	V	89	GLN	2.8
12	W	13	THR	2.7
1	A	122	GLN	2.7
8	S	7	LYS	2.7
2	B	33	VAL	2.7
6	Q	74	VAL	2.7
7	G	19	PRO	2.7
11	V	63	SER	2.7
1	L	30	THR	2.7
12	W	56	ALA	2.7
10	J	89	GLU	2.7
2	B	335	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
6	Q	103	GLU	2.7
2	B	256	LEU	2.7
12	W	30	PRO	2.7
8	H	87	GLU	2.7
8	H	50	ARG	2.7
8	H	86	ARG	2.7
9	I	3	PHE	2.7
11	V	26	SER	2.7
7	G	17	LYS	2.6
10	J	55	VAL	2.6
10	J	1	GLU	2.6
5	P	102	PRO	2.6
1	A	111	GLY	2.6
2	M	328	GLN	2.6
2	M	248	ALA	2.6
1	A	235	LYS	2.6
1	L	228	LEU	2.6
2	M	31	LEU	2.6
2	B	217	SER	2.6
12	W	81	PRO	2.6
8	H	2	GLY	2.6
11	V	19	VAL	2.6
5	P	154	ILE	2.6
11	K	33	LEU	2.6
12	W	105	LYS	2.6
11	K	2	ILE	2.6
5	E	40	ASP	2.6
1	A	221	ASN	2.5
10	U	1	GLU	2.5
5	P	99	ALA	2.5
7	G	90	ARG	2.5
10	U	103	SER	2.5
2	B	220	GLU	2.5
11	K	13	ALA	2.5
2	M	256	LEU	2.5
11	V	2	ILE	2.5
10	J	83	LEU	2.5
1	A	226	LYS	2.5
1	L	122	GLN	2.5
5	P	124	HIS	2.5
1	A	238	LEU	2.5
2	M	17	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
5	P	123	PRO	2.5
11	V	61	ARG	2.5
2	B	318	ILE	2.5
10	U	122	SER	2.5
10	U	68	LEU	2.5
7	R	19	PRO	2.5
5	E	97	ASN	2.4
5	P	212	VAL	2.4
1	A	218	ASP	2.4
6	Q	114	TYR	2.4
1	A	115	LYS	2.4
5	P	103	LEU	2.4
10	J	3	LYS	2.4
1	L	237	VAL	2.4
10	J	57	ASP	2.4
4	O	307	PRO	2.4
6	F	114	TYR	2.4
6	F	97	HIS	2.4
1	A	401	LEU	2.4
1	A	114	ASP	2.4
9	I	26	PHE	2.4
2	M	292	GLN	2.4
4	D	307	PRO	2.4
2	M	219	SER	2.4
10	J	66	ASP	2.4
1	L	72	LEU	2.4
11	V	87	PHE	2.4
1	A	118	ASP	2.4
9	I	9	THR	2.4
10	J	49	VAL	2.4
11	K	32	PHE	2.4
12	W	3	PHE	2.4
11	V	67	SER	2.4
11	V	102	THR	2.4
7	R	126	SER	2.3
2	B	343	VAL	2.3
6	Q	110	GLN	2.3
6	F	113	GLY	2.3
1	L	401	LEU	2.3
11	K	76	SER	2.3
11	V	51	THR	2.3
1	L	381	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
4	O	137	GLU	2.3
11	K	83	ILE	2.3
1	L	45	SER	2.3
5	P	31	LYS	2.3
11	V	40	PRO	2.3
10	J	81	LEU	2.3
2	M	187	VAL	2.3
1	A	34	ASN	2.3
11	V	76	SER	2.3
5	E	118	ILE	2.3
4	D	209	PRO	2.3
11	K	22	SER	2.3
5	P	105	LYS	2.3
9	T	56	ILE	2.3
11	V	97	THR	2.3
2	M	22	ARG	2.2
11	K	4	LEU	2.2
2	M	25	PRO	2.2
2	M	213	LYS	2.2
6	Q	113	GLY	2.2
11	K	89	GLN	2.2
12	W	8	ALA	2.2
2	B	345	ASP	2.2
12	W	29	GLY	2.2
8	H	91	ARG	2.2
4	D	62	MET	2.2
1	A	217	GLU	2.2
12	W	6	GLY	2.2
10	U	88	THR	2.2
8	S	56	PHE	2.2
11	K	39	LYS	2.2
1	L	219	LEU	2.2
6	Q	75	THR	2.2
11	V	22	SER	2.2
1	L	111	GLY	2.2
10	J	44	ASN	2.2
1	A	224	GLU	2.2
4	O	141	GLN	2.2
12	W	99	LEU	2.2
2	M	327	VAL	2.2
1	A	278	ALA	2.1
4	D	135	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
4	D	200	ASP	2.1
5	P	145	ASP	2.1
10	J	8	GLY	2.1
8	S	67	TRP	2.1
1	A	36	ILE	2.1
1	A	134	SER	2.1
2	M	220	GLU	2.1
6	F	110	GLN	2.1
4	D	185	HIS	2.1
11	K	18	ARG	2.1
2	B	310	LYS	2.1
2	M	310	LYS	2.1
8	H	67	TRP	2.1
2	B	340	PHE	2.1
11	K	63	SER	2.1
2	M	345	ASP	2.1
8	S	68	TYR	2.1
10	U	3	LYS	2.1
10	U	125	ARG	2.1
2	B	187	VAL	2.1
10	U	49	VAL	2.1
7	G	10	ARG	2.1
11	V	57	GLY	2.1
11	V	99	GLY	2.1
2	B	155	LEU	2.1
2	B	246	ASN	2.1
7	G	97	GLN	2.1
2	M	334	SER	2.1
8	S	90	GLU	2.1
1	L	76	ILE	2.1
5	E	213	ILE	2.1
5	P	152	TRP	2.1
1	A	72	LEU	2.1
2	B	197	LEU	2.1
2	M	239	ALA	2.1
6	Q	117	LEU	2.1
6	Q	130	LEU	2.1
11	K	54	LEU	2.1
11	V	1	ASP	2.1
7	R	90	ARG	2.1
10	J	74	THR	2.1
11	K	97	THR	2.1

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Mol	Chain	Res	Type	RSRZ
2	M	335	PRO	2.1
5	E	48	ASP	2.1
2	M	340	PHE	2.0
10	J	41	PHE	2.0
11	K	12	ALA	2.0
11	V	44	ILE	2.0
1	L	343	LEU	2.0
9	T	6	LEU	2.0
11	K	8	PRO	2.0
10	U	18	LEU	2.0
10	U	16	GLN	2.0
10	U	85	SER	2.0
2	B	341	ASP	2.0
4	O	239	GLY	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	77	12/13	0.86	0.32	-	64,68,72,72	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
20	CN5	C	4033	41/41	0.63	0.23	7.68	76,79,85,86	0
18	8PE	N	4110	47/47	0.82	0.17	2.51	43,51,65,67	0
21	7PH	O	4114	38/38	0.94	0.15	2.15	40,44,52,52	0
21	7PH	D	4014	38/38	0.94	0.16	2.10	43,46,62,63	0
19	9PE	N	4111	40/40	0.91	0.13	2.04	39,47,62,66	0
19	9PE	C	4011	40/40	0.93	0.13	1.58	39,46,70,72	0
14	6PH	L	4113	40/40	0.86	0.14	1.13	51,55,67,68	0
14	6PH	A	4013	40/40	0.89	0.13	1.01	48,55,61,61	0
22	CN3	N	4131	55/55	0.90	0.16	0.90	39,58,66,69	0
13	SUC	O	4146	23/23	0.73	0.23	0.90	68,70,73,76	0
16	HEM	D	4003	43/43	0.97	0.12	0.70	23,29,33,34	0
22	CN3	D	4031	55/55	0.86	0.18	0.49	48,62,70,71	0
18	8PE	C	4010	47/47	0.81	0.16	0.46	39,50,59,60	0
17	SMA	N	4025	37/37	0.95	0.11	0.36	21,24,30,33	0
17	SMA	C	4005	37/37	0.95	0.11	0.12	22,24,31,34	0
16	HEM	N	4022	43/43	0.98	0.10	0.03	15,18,26,28	0
16	HEM	W	4026	43/43	0.92	0.15	-0.13	46,50,54,55	0
16	HEM	O	4023	43/43	0.98	0.09	-0.25	25,28,30,33	0
15	UMQ	A	4021	34/34	0.94	0.11	-0.28	32,36,55,56	0
16	HEM	C	4001	43/43	0.99	0.09	-0.29	16,21,26,30	0
16	HEM	C	4002	43/43	0.99	0.08	-0.49	17,20,24,28	0
15	UMQ	L	4121	34/34	0.94	0.10	-0.55	33,35,57,58	0
16	HEM	N	4021	43/43	0.98	0.08	-0.65	16,20,25,27	0
23	FES	P	4024	4/4	0.99	0.09	-0.85	28,29,31,32	0
23	FES	E	4004	4/4	0.99	0.07	-1.54	27,27,28,31	0

6.5 Other polymers (i)

There are no such residues in this entry.