



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2018 – 02:13 pm 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 wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

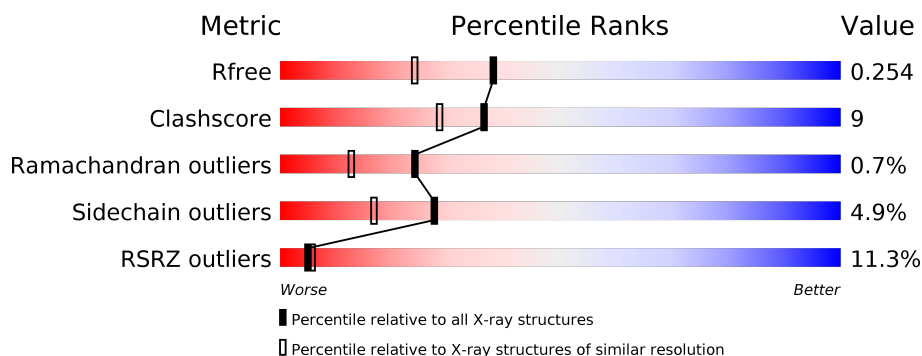
1 Overall quality at a glance

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}	111664	5502 (1.90-1.90)
Clashscore	122126	6115 (1.90-1.90)
Ramachandran outliers	120053	6048 (1.90-1.90)
Sidechain outliers	120020	6048 (1.90-1.90)
RSRZ outliers	108989	5379 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	431	<div> <div>12%</div> <div>79%</div> <div>19%</div> <div>.</div> </div>
1	L	431	<div> <div>9%</div> <div>76%</div> <div>20%</div> <div>.</div> </div>
2	B	352	<div> <div>8%</div> <div>76%</div> <div>22%</div> <div>.</div> </div>
2	M	352	<div> <div>10%</div> <div>72%</div> <div>25%</div> <div>.</div> </div>
3	C	385	<div> <div>%</div> <div>84%</div> <div>15%</div> <div>.</div> </div>
3	N	385	<div> <div>%</div> <div>84%</div> <div>15%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
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	

2 Entry composition [i](#)

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			

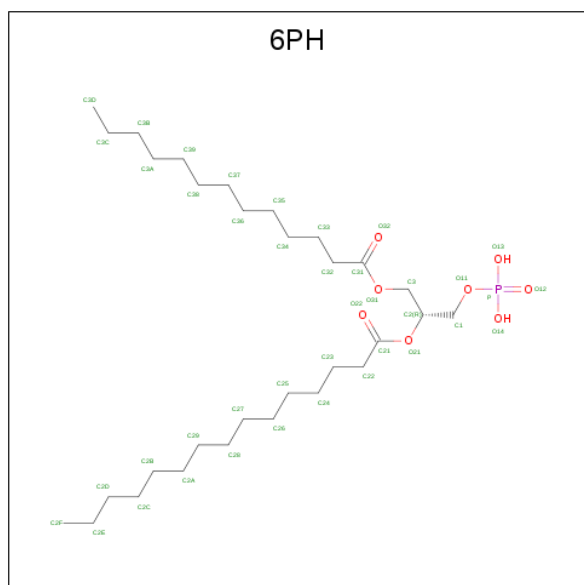
- Molecule 11 is a protein called LIGHT CHAIN (VL) OF FV-FRAGMENT.

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 (1R)-2-(phosphonoxy)-1-[(tridecanoyloxy)methyl]ethyl pentadecanoate (three-letter code: 6PH) (formula: C₃₁H₆₁O₈P).



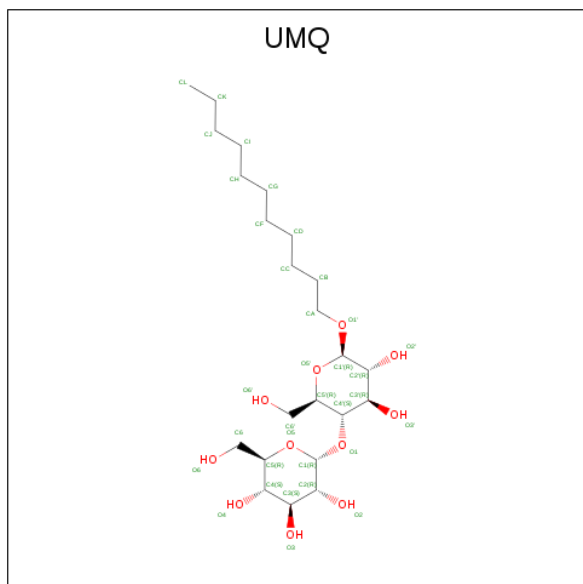
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	A	1	Total	C	O	P	0	0
			40	31	8	1		

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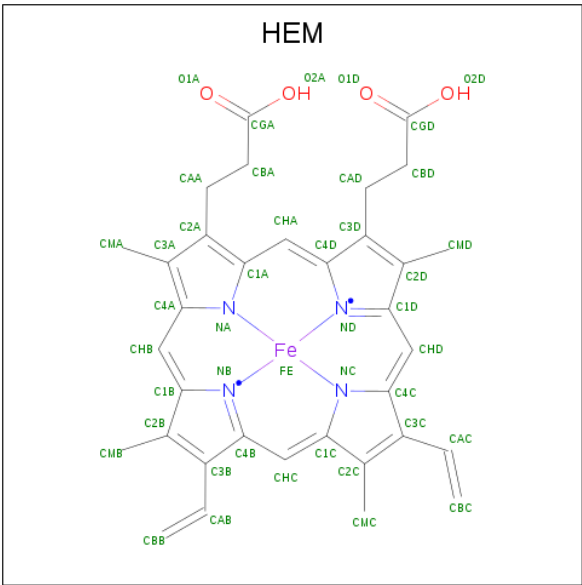
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	L	1	Total	C	O	P	0	0
			40	31	8	1		

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



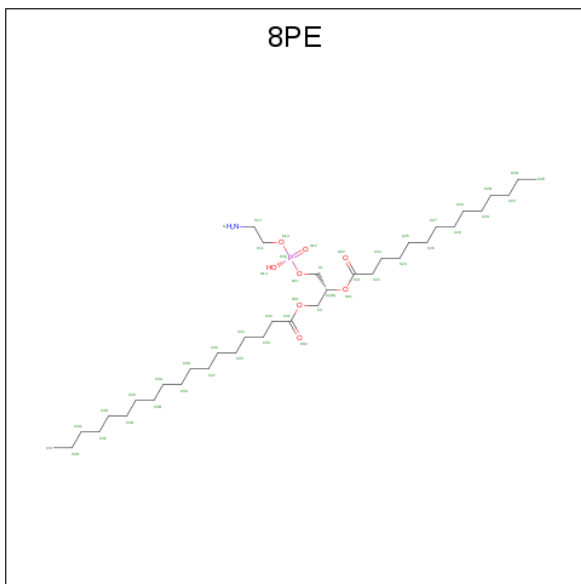
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	A	1	Total	C	O		0	0
			34	23	11			
14	L	1	Total	C	O		0	0
			34	23	11			

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



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

- Molecule 16 is STIGMATELLIN A (three-letter code: SMA) (formula: C₃₀H₄₂O₇).



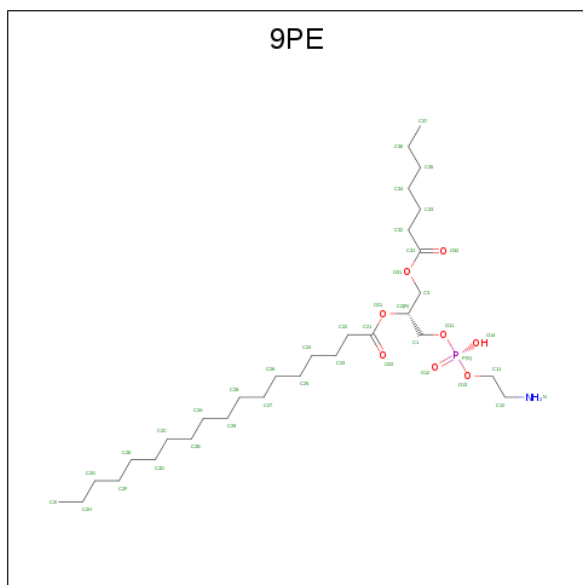
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	C	1	Total 47	C 37	N 1	O 8	P 1	0	0

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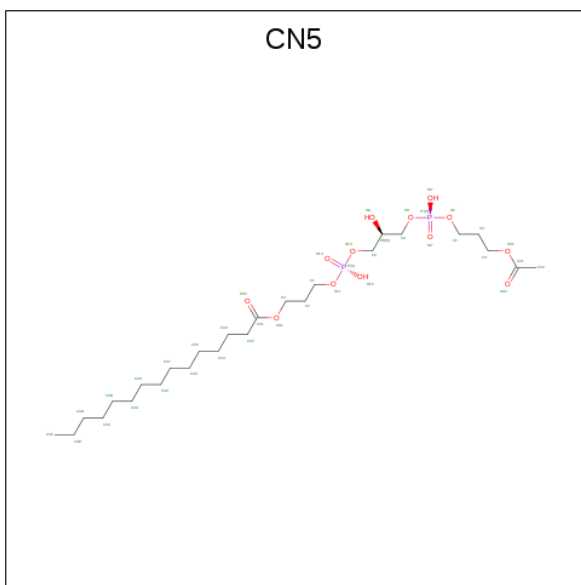
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	N	1	Total	C	N	O	P	0	0
			47	37	1	8	1		

- Molecule 18 is (1R)-2-{[(S)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-1-[(heptanoyloxy)methyl]ethyl octadecanoate (three-letter code: 9PE) (formula: C₃₀H₆₀NO₈P).



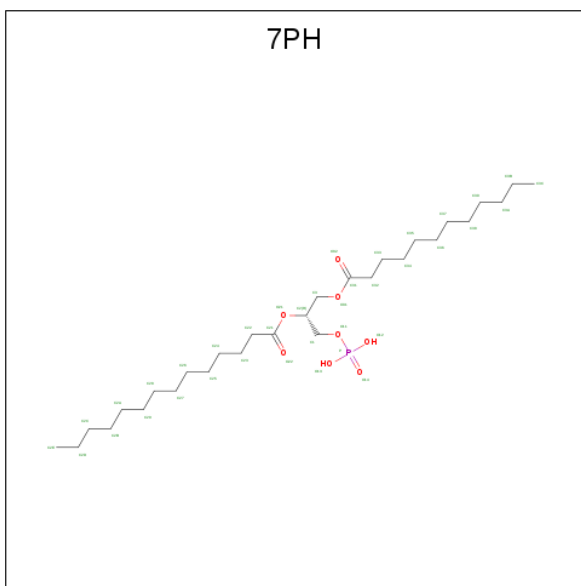
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	C	1	Total	C	N	O	P	0	0
			40	30	1	8	1		
18	N	1	Total	C	N	O	P	0	0
			40	30	1	8	1		

- Molecule 19 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: C₂₆H₅₂O₁₃P₂).



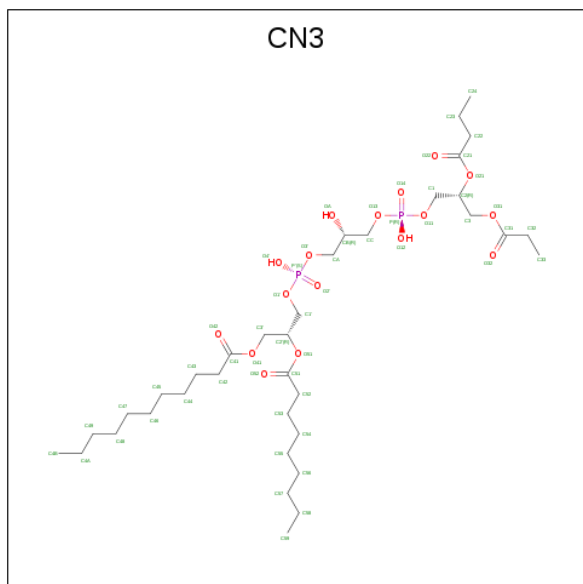
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	C	1	Total	C	O	P	0	0
			41	26	13	2		

- Molecule 20 is (1R)-2-(dodecanoyloxy)-1-[(phosphonooxy)methyl]ethyl tetradecanoate (three-letter code: 7PH) (formula: $C_{29}H_{57}O_8P$).



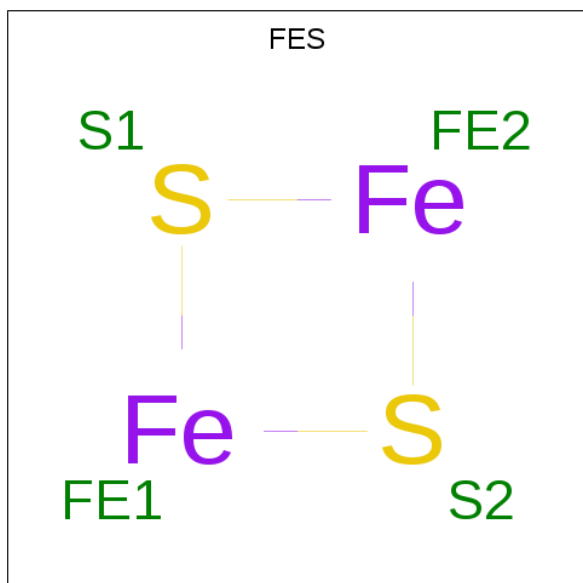
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	D	1	Total	C	O	P	0	0
			38	29	8	1		
20	O	1	Total	C	O	P	0	0
			38	29	8	1		

- Molecule 21 is (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-diphosphanadec-1-yl undecanoate (three-letter code: CN3) (formula: $C_{36}H_{68}O_{17}P_2$).



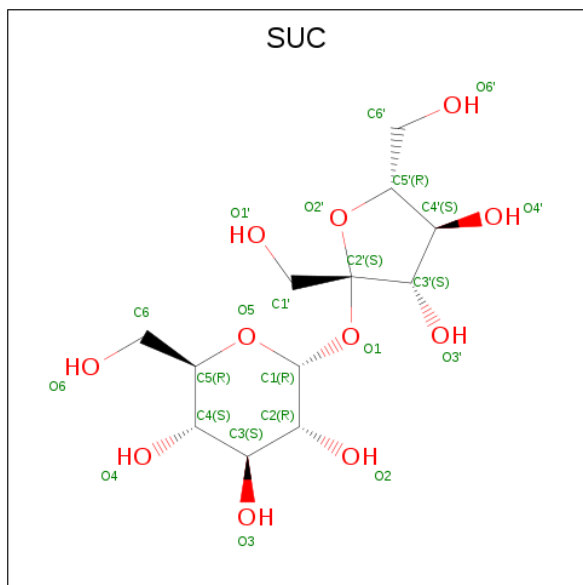
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
21	D	1	Total	C	O	P	0	0
			55	36	17	2		
21	N	1	Total	C	O	P	0	0
			55	36	17	2		

- Molecule 22 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



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

- Molecule 23 is SUCROSE (three-letter code: SUC) (formula: $C_{12}H_{22}O_{11}$).



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

- Molecule 24 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	A	153	Total	O	0	0
			153	153		
24	B	93	Total	O	0	0
			93	93		
24	C	161	Total	O	0	0
			161	161		
24	D	154	Total	O	0	0
			154	154		
24	E	74	Total	O	0	0
			74	74		
24	F	16	Total	O	0	0
			16	16		
24	G	71	Total	O	0	0
			71	71		

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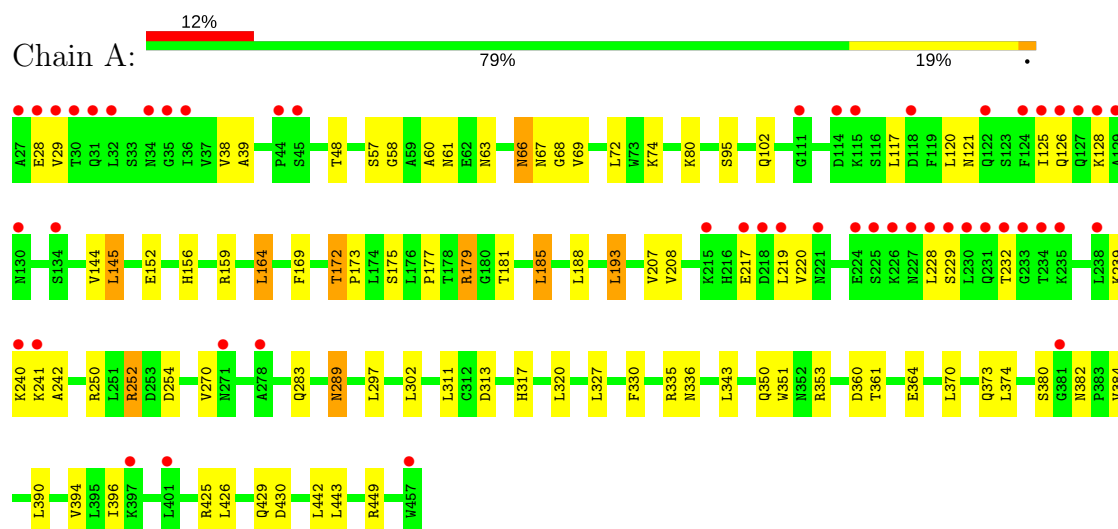
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	H	31	Total 31	O 31	0	0
24	I	11	Total 11	O 11	0	0
24	J	15	Total 15	O 15	0	0
24	K	7	Total 7	O 7	0	0
24	L	170	Total 170	O 170	0	0
24	M	101	Total 101	O 101	0	0
24	N	170	Total 170	O 170	0	0
24	O	173	Total 173	O 173	0	0
24	P	66	Total 66	O 66	0	0
24	Q	27	Total 27	O 27	0	0
24	R	73	Total 73	O 73	0	0
24	S	40	Total 40	O 40	0	0
24	T	12	Total 12	O 12	0	0
24	U	8	Total 8	O 8	0	0
24	V	2	Total 2	O 2	0	0
24	W	20	Total 20	O 20	0	0

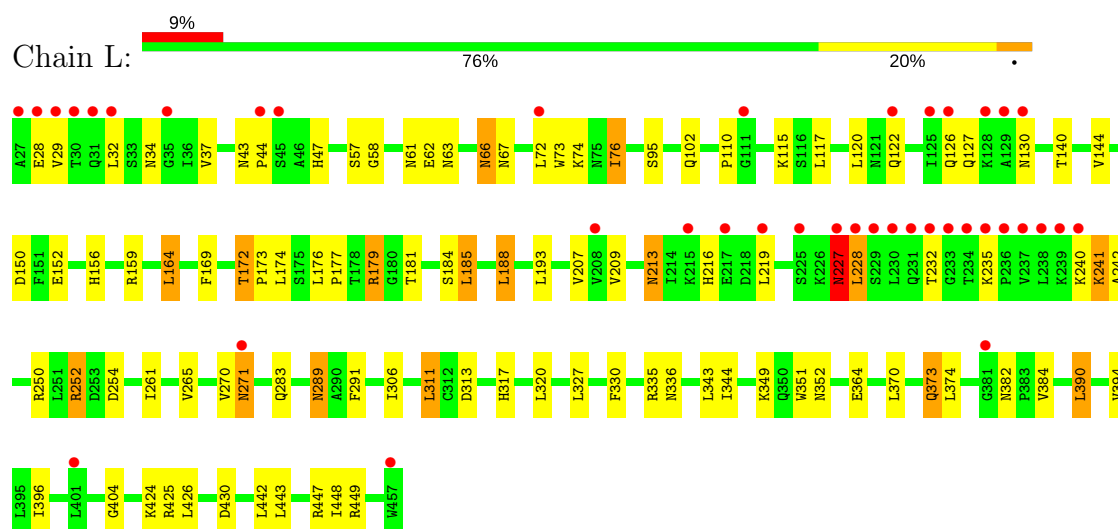
3 Residue-property plots [i](#)

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

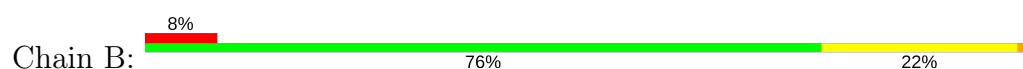
- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial

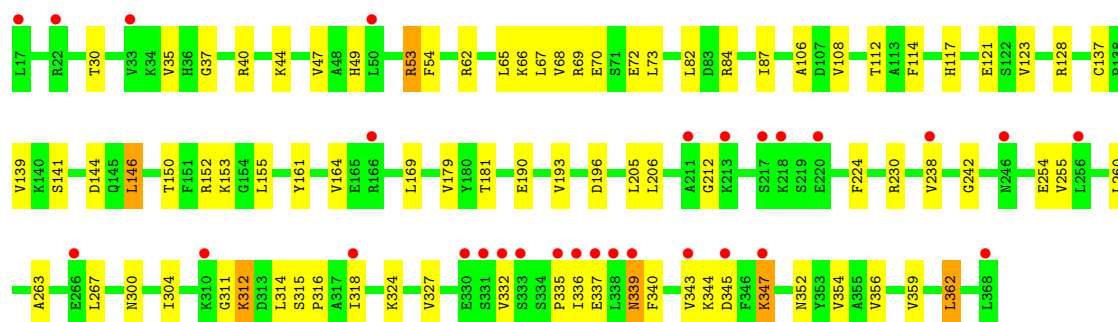


- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial

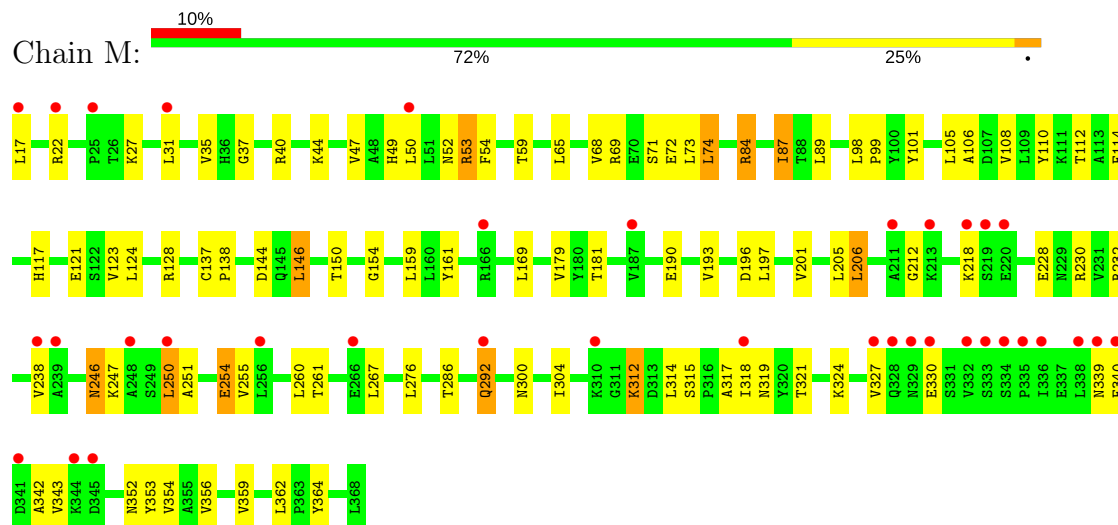


- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

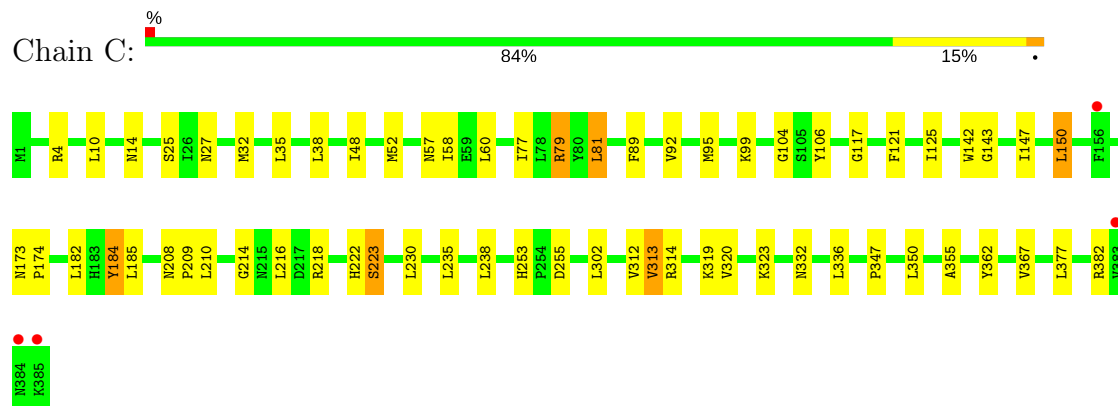




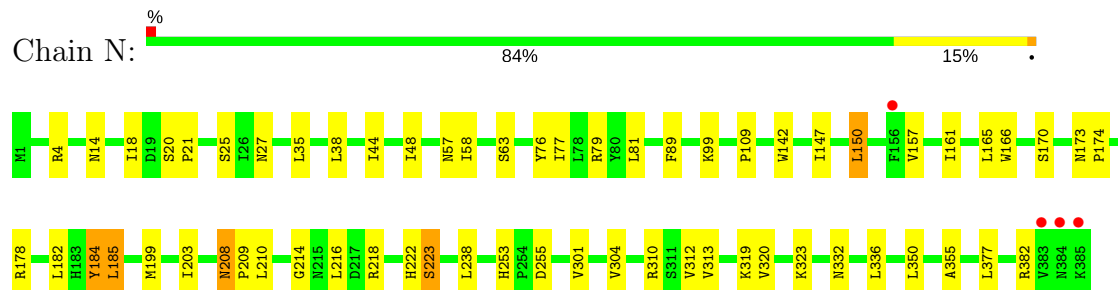
• Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial



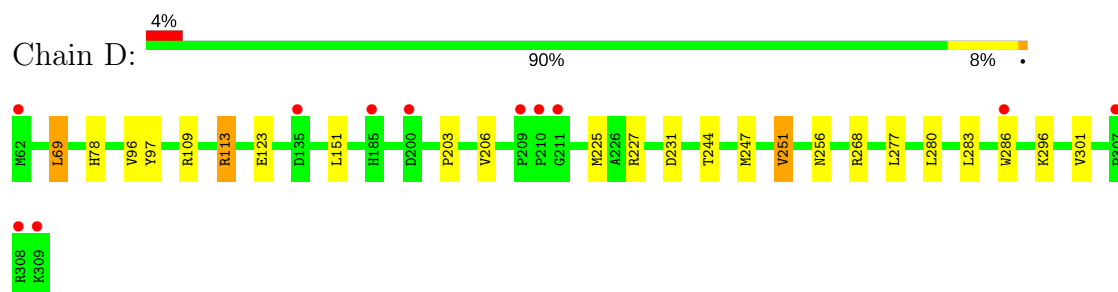
• Molecule 3: CYTOCHROME B



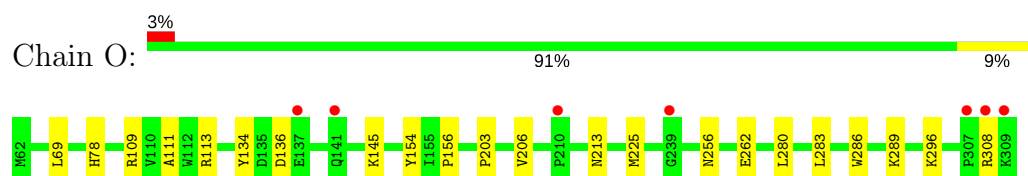
• Molecule 3: CYTOCHROME B



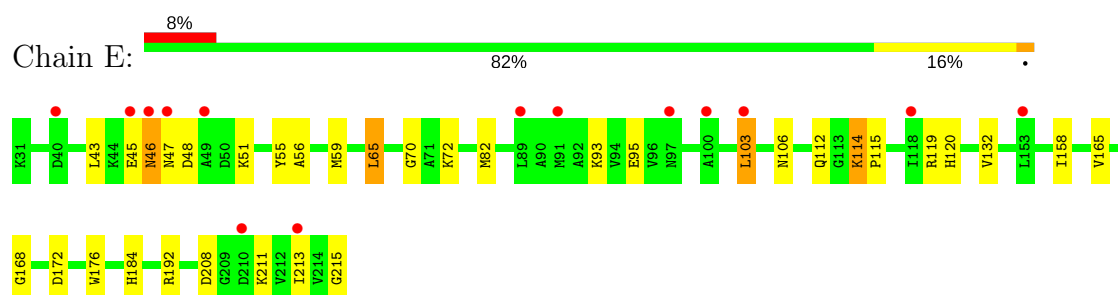
- Molecule 4: Cytochrome c1, heme protein, mitochondrial



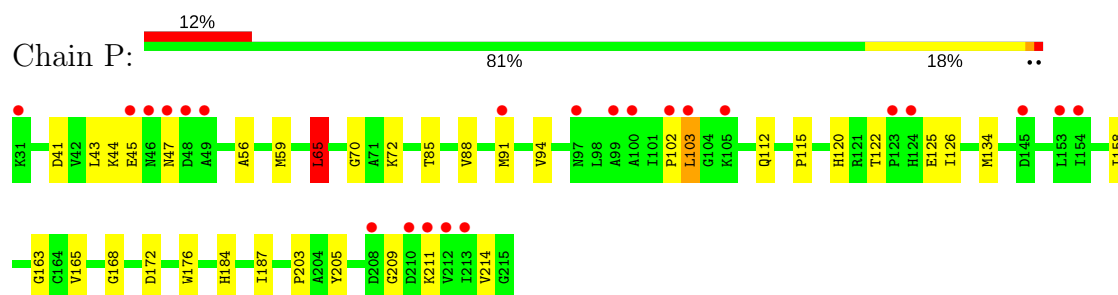
- Molecule 4: Cytochrome c1, heme protein, mitochondrial



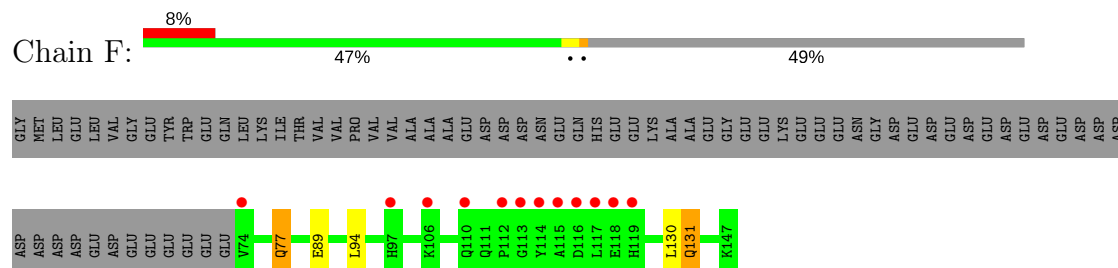
- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial



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




- Molecule 6: Cytochrome b-c1 complex subunit 6




- Molecule 6: Cytochrome b-c1 complex subunit 6

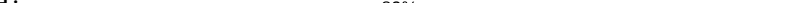


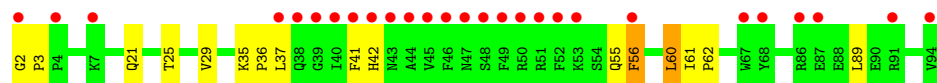
- Chain G:  6% 79% 18%



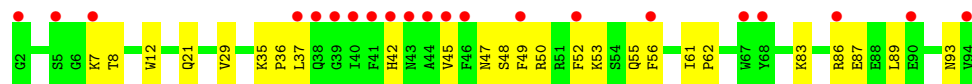
- Chain R:  5% 79% 20%

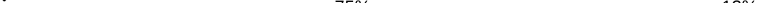


- Chain H: 



- Chain S: 



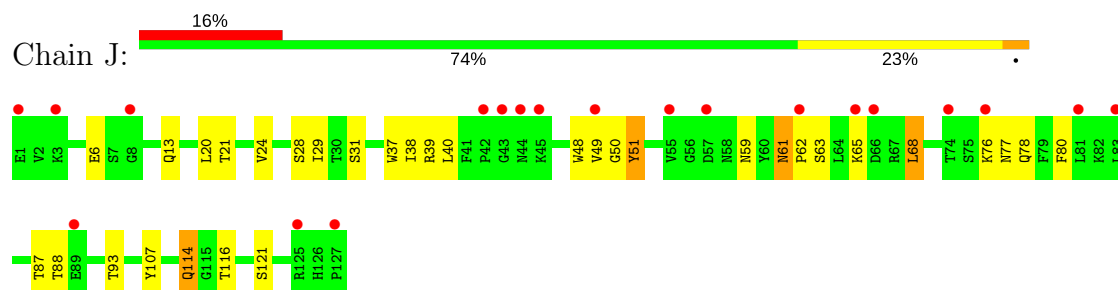
- Chain I: 



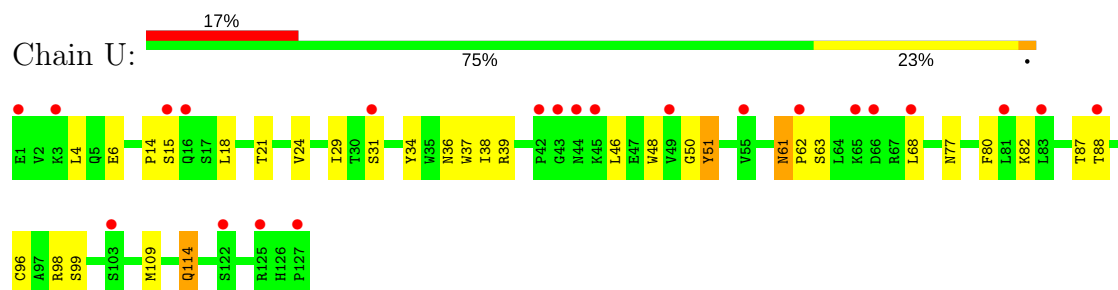
- Chain T:  11% 72% 14% 12%



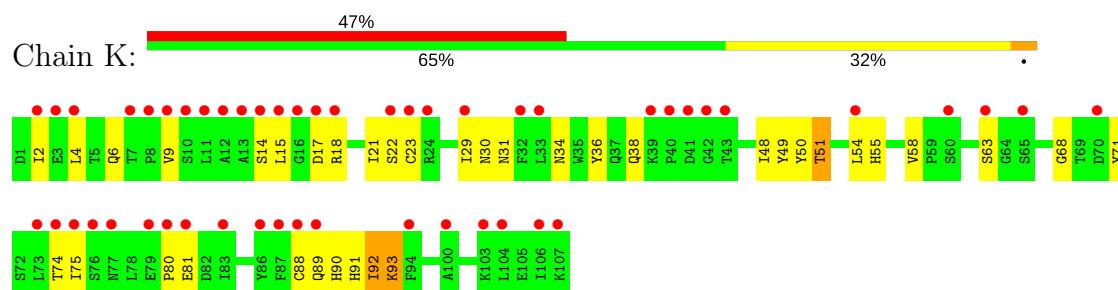
- Molecule 10: HEAVY CHAIN (VH) OF FV-FRAGMENT



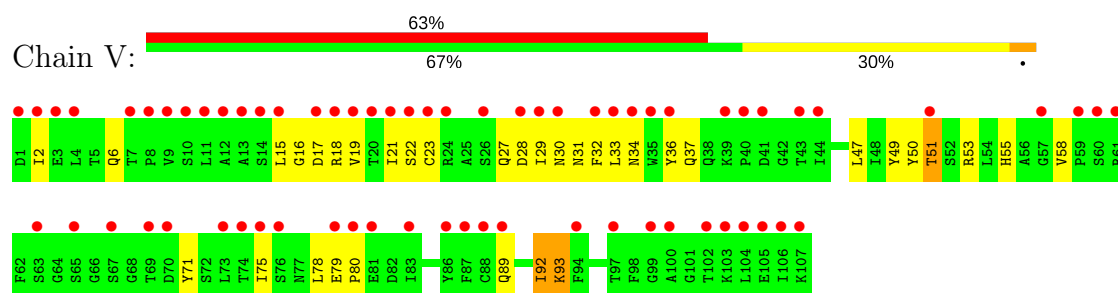
- Molecule 10: HEAVY CHAIN (VH) OF FV-FRAGMENT



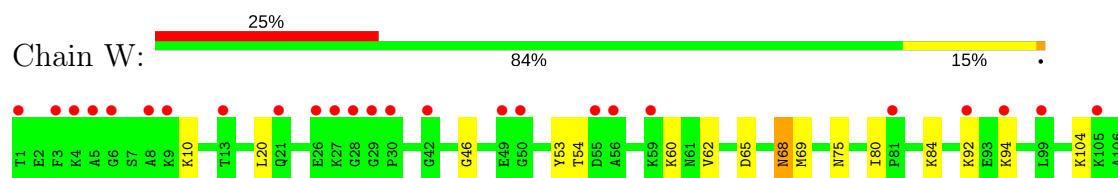
- Molecule 11: LIGHT CHAIN (VL) OF FV-FRAGMENT



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



- Molecule 12: Cytochrome c iso-1





4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 1.90Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.245 , 0.263 0.238 , 0.254	Depositor DCC
R_{free} test set	33007 reflections (5.00%)	wwPDB-VP
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
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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

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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	A	40	0	59	1	0
13	L	40	0	59	3	0
14	A	34	0	44	2	0
14	L	34	0	44	2	0
15	C	86	0	60	2	0
15	D	43	0	30	1	0
15	N	86	0	60	3	0
15	O	43	0	30	0	0
15	W	43	0	30	0	0
16	C	37	0	42	1	0
16	N	37	0	42	0	0
17	C	47	0	73	1	0
17	N	47	0	73	0	0
18	C	40	0	59	0	0
18	N	40	0	59	0	0
19	C	41	0	50	5	0
20	D	38	0	55	2	0
20	O	38	0	55	2	0
21	D	55	0	66	5	0
21	N	55	0	66	5	0
22	E	4	0	0	0	0
22	P	4	0	0	0	0
23	O	23	0	22	5	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

The worst 5 of 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
6:F:77:GLN:HE21	6:F:77:GLN:H	1.12	0.97
2:M:150:THR:HG22	2:M:352:ASN:HD22	1.27	0.97
2:M:255:VAL:HG12	2:M:321:THR:HG21	1.47	0.96

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%)	31	20
1	L	429/431 (100%)	406 (95%)	19 (4%)	4 (1%)	19	8
2	B	350/352 (99%)	330 (94%)	15 (4%)	5 (1%)	12	3
2	M	350/352 (99%)	330 (94%)	19 (5%)	1 (0%)	43	33
3	C	383/385 (100%)	370 (97%)	12 (3%)	1 (0%)	43	33
3	N	383/385 (100%)	369 (96%)	13 (3%)	1 (0%)	43	33
4	D	246/248 (99%)	238 (97%)	8 (3%)	0	100	100
4	O	246/248 (99%)	241 (98%)	4 (2%)	1 (0%)	36	25
5	E	183/185 (99%)	173 (94%)	8 (4%)	2 (1%)	16	5
5	P	183/185 (99%)	169 (92%)	10 (6%)	4 (2%)	7	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%)	16	5
8	S	91/93 (98%)	83 (91%)	7 (8%)	1 (1%)	16	5
9	I	55/65 (85%)	53 (96%)	2 (4%)	0	100	100
9	T	55/65 (85%)	52 (94%)	2 (4%)	1 (2%)	9	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%)	3	0
11	V	105/107 (98%)	91 (87%)	11 (10%)	3 (3%)	5	1
12	W	106/108 (98%)	104 (98%)	2 (2%)	0	100	100
All	All	4432/4638 (96%)	4206 (95%)	195 (4%)	31 (1%)	24	13

5 of 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

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%)	15	6
1	L	370/370 (100%)	340 (92%)	30 (8%)	13	5
2	B	301/301 (100%)	288 (96%)	13 (4%)	32	21
2	M	301/301 (100%)	282 (94%)	19 (6%)	20	9
3	C	338/338 (100%)	318 (94%)	20 (6%)	21	11
3	N	338/338 (100%)	321 (95%)	17 (5%)	27	16
4	D	206/206 (100%)	200 (97%)	6 (3%)	45	37
4	O	206/206 (100%)	202 (98%)	4 (2%)	60	55
5	E	151/151 (100%)	149 (99%)	2 (1%)	71	70
5	P	151/151 (100%)	146 (97%)	5 (3%)	41	32
6	F	67/130 (52%)	62 (92%)	5 (8%)	15	6
6	Q	67/130 (52%)	63 (94%)	4 (6%)	21	11
7	G	110/110 (100%)	105 (96%)	5 (4%)	30	20
7	R	110/110 (100%)	107 (97%)	3 (3%)	48	40
8	H	77/77 (100%)	74 (96%)	3 (4%)	35	25
8	S	77/77 (100%)	76 (99%)	1 (1%)	71	70
9	I	47/53 (89%)	46 (98%)	1 (2%)	56	51
9	T	47/53 (89%)	45 (96%)	2 (4%)	32	21
10	J	112/112 (100%)	105 (94%)	7 (6%)	20	9
10	U	112/112 (100%)	107 (96%)	5 (4%)	30	20
11	K	93/93 (100%)	88 (95%)	5 (5%)	24	14
11	V	93/93 (100%)	90 (97%)	3 (3%)	42	33
12	W	89/88 (101%)	87 (98%)	2 (2%)	55	49
All	All	3833/3970 (96%)	3644 (95%)	189 (5%)	27	17

5 of 189 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	J	59	ASN
1	L	188	LEU
7	R	16	LEU
10	J	114	GLN
1	L	76	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 131 such sidechains are listed below:

Mol	Chain	Res	Type
11	K	89	GLN
1	L	170	GLN
10	U	114	GLN
11	K	91	HIS
1	L	67	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	11,11,12	1.08	1 (9%)	11,14,16	1.04	1 (9%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	M3L	W	77	12	-	0/8/10/12	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	W	77	M3L	CA-C	2.16	1.53	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	W	77	M3L	CM2-NZ-CM1	-2.10	103.64	108.96

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
13	6PH	A	4013	-	39,39,39	0.99	2 (5%)	43,44,44	1.47	5 (11%)
14	UMQ	A	4021	-	35,35,35	0.91	1 (2%)	46,46,46	1.76	7 (15%)
15	HEM	C	4001	3	27,50,50	1.72	6 (22%)	17,82,82	1.00	0
15	HEM	C	4002	3	27,50,50	1.62	7 (25%)	17,82,82	1.26	2 (11%)
16	SMA	C	4005	-	36,38,38	1.27	3 (8%)	44,52,52	1.52	6 (13%)
17	8PE	C	4010	-	46,46,46	0.95	2 (4%)	49,51,51	1.18	3 (6%)
18	9PE	C	4011	-	39,39,39	0.70	0	42,44,44	0.96	1 (2%)
19	CN5	C	4033	-	40,40,40	1.61	9 (22%)	44,48,48	1.85	8 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	HEM	D	4003	4	27,50,50	1.67	6 (22%)	17,82,82	0.94	0
20	7PH	D	4014	-	37,37,37	0.98	1 (2%)	41,42,42	1.57	9 (21%)
21	CN3	D	4031	-	54,54,54	1.51	10 (18%)	60,66,66	1.53	7 (11%)
22	FES	E	4004	5	0,4,4	0.00	-	0,4,4	0.00	-
13	6PH	L	4113	-	39,39,39	1.00	2 (5%)	43,44,44	1.51	5 (11%)
14	UMQ	L	4121	-	35,35,35	0.94	1 (2%)	46,46,46	1.73	5 (10%)
15	HEM	N	4021	3	27,50,50	1.78	7 (25%)	17,82,82	1.05	1 (5%)
15	HEM	N	4022	3	27,50,50	1.66	8 (29%)	17,82,82	1.17	2 (11%)
16	SMA	N	4025	-	36,38,38	1.25	4 (11%)	44,52,52	1.61	7 (15%)
17	8PE	N	4110	-	46,46,46	0.99	4 (8%)	49,51,51	1.14	2 (4%)
18	9PE	N	4111	-	39,39,39	0.74	0	42,44,44	0.99	1 (2%)
21	CN3	N	4131	-	54,54,54	1.48	10 (18%)	60,66,66	1.51	7 (11%)
15	HEM	O	4023	4	27,50,50	1.76	6 (22%)	17,82,82	1.21	1 (5%)
20	7PH	O	4114	-	37,37,37	0.98	2 (5%)	41,42,42	1.57	9 (21%)
23	SUC	O	4146	-	24,24,24	0.53	0	36,36,36	0.70	1 (2%)
22	FES	P	4024	5	0,4,4	0.00	-	0,4,4	0.00	-
15	HEM	W	4026	12	27,50,50	1.64	6 (22%)	17,82,82	1.18	1 (5%)

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
13	6PH	A	4013	-	-	0/41/41/41	0/0/0/0
14	UMQ	A	4021	-	-	0/20/60/60	0/2/2/2
15	HEM	C	4001	3	-	0/6/54/54	0/0/8/8
15	HEM	C	4002	3	-	0/6/54/54	0/0/8/8
16	SMA	C	4005	-	-	0/33/34/34	0/2/2/2
17	8PE	C	4010	-	-	0/50/50/50	0/0/0/0
18	9PE	C	4011	-	-	0/43/43/43	0/0/0/0
19	CN5	C	4033	-	-	0/44/44/44	0/0/0/0
15	HEM	D	4003	4	-	0/6/54/54	0/0/8/8
20	7PH	D	4014	-	-	0/39/39/39	0/0/0/0
21	CN3	D	4031	-	-	0/65/65/65	0/0/0/0
22	FES	E	4004	5	-	0/0/4/4	0/1/1/1
13	6PH	L	4113	-	-	0/41/41/41	0/0/0/0
14	UMQ	L	4121	-	-	0/20/60/60	0/2/2/2
15	HEM	N	4021	3	-	0/6/54/54	0/0/8/8

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	HEM	N	4022	3	-	0/6/54/54	0/0/8/8
16	SMA	N	4025	-	-	0/33/34/34	0/2/2/2
17	8PE	N	4110	-	-	0/50/50/50	0/0/0/0
18	9PE	N	4111	-	-	0/43/43/43	0/0/0/0
21	CN3	N	4131	-	-	0/65/65/65	0/0/0/0
15	HEM	O	4023	4	-	0/6/54/54	0/0/8/8
20	7PH	O	4114	-	-	0/39/39/39	0/0/0/0
23	SUC	O	4146	-	-	0/12/51/51	0/2/2/2
22	FES	P	4024	5	-	0/0/4/4	0/1/1/1
15	HEM	W	4026	12	-	0/6/54/54	0/0/8/8

The worst 5 of 97 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	D	4031	CN3	O31-C3	-4.44	1.35	1.45
21	N	4131	CN3	O31-C3	-4.43	1.35	1.45
15	C	4001	HEM	C3C-CAC	-4.14	1.39	1.47
15	N	4021	HEM	C3C-CAC	-4.10	1.39	1.47
15	N	4021	HEM	C3B-CAB	-3.83	1.40	1.47

The worst 5 of 90 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	4021	UMQ	CA-O1'-C1'	-8.72	98.95	113.85
14	L	4121	UMQ	CA-O1'-C1'	-8.44	99.44	113.85
21	D	4031	CN3	C2'-O51-C51	-5.44	105.03	117.88
21	N	4131	CN3	C2'-O51-C51	-5.19	105.60	117.88
16	C	4005	SMA	C3-C4-C4A	-5.01	114.60	121.25

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
13	A	4013	6PH	1	0
14	A	4021	UMQ	2	0
15	C	4001	HEM	1	0
15	C	4002	HEM	1	0
16	C	4005	SMA	1	0
17	C	4010	8PE	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	C	4033	CN5	5	0
15	D	4003	HEM	1	0
20	D	4014	7PH	2	0
21	D	4031	CN3	5	0
13	L	4113	6PH	3	0
14	L	4121	UMQ	2	0
15	N	4021	HEM	2	0
15	N	4022	HEM	1	0
21	N	4131	CN3	5	0
20	O	4114	7PH	2	0
23	O	4146	SUC	5	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	431/431 (100%)	0.54	50 (11%) 4 5	26, 44, 98, 114	0
1	L	431/431 (100%)	0.46	40 (9%) 8 10	25, 42, 90, 113	0
2	B	352/352 (100%)	0.59	29 (8%) 11 13	30, 47, 73, 114	0
2	M	352/352 (100%)	0.54	36 (10%) 7 8	32, 45, 72, 109	0
3	C	385/385 (100%)	-0.17	4 (1%) 82 84	18, 27, 38, 91	0
3	N	385/385 (100%)	-0.22	4 (1%) 82 84	19, 26, 37, 88	0
4	D	248/248 (100%)	0.00	11 (4%) 34 37	25, 35, 57, 83	0
4	O	248/248 (100%)	-0.05	7 (2%) 53 56	24, 33, 55, 86	0
5	E	185/185 (100%)	0.45	14 (7%) 14 15	24, 40, 69, 94	0
5	P	185/185 (100%)	0.65	23 (12%) 4 4	24, 41, 80, 93	0
6	F	74/146 (50%)	0.82	12 (16%) 1 1	34, 46, 90, 96	0
6	Q	74/146 (50%)	0.78	13 (17%) 1 1	32, 45, 87, 90	0
7	G	126/126 (100%)	-0.04	7 (5%) 24 28	26, 37, 60, 78	0
7	R	126/126 (100%)	-0.02	6 (4%) 30 34	23, 34, 62, 80	0
8	H	93/93 (100%)	1.85	27 (29%) 0 0	24, 45, 128, 131	0
8	S	93/93 (100%)	1.29	21 (22%) 0 0	22, 43, 113, 119	0
9	I	57/65 (87%)	0.83	7 (12%) 4 4	34, 42, 83, 100	0
9	T	57/65 (87%)	0.76	7 (12%) 4 4	32, 40, 84, 96	0
10	J	127/127 (100%)	0.93	20 (15%) 2 2	40, 57, 71, 80	0
10	U	127/127 (100%)	1.12	22 (17%) 1 1	42, 59, 73, 82	0
11	K	107/107 (100%)	2.27	50 (46%) 0 0	51, 81, 114, 116	0
11	V	107/107 (100%)	2.82	67 (62%) 0 0	60, 92, 120, 122	0
12	W	107/108 (99%)	1.43	27 (25%) 0 0	46, 62, 87, 99	0
All	All	4477/4638 (96%)	0.52	504 (11%) 5 6	18, 41, 90, 131	0

The worst 5 of 504 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
8	H	46	PHE	19.6
2	B	338	LEU	18.4
1	L	230	LEU	17.9
9	I	57	ALA	13.6
9	T	58	ALA	13.5

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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
19	CN5	C	4033	41/41	0.63	0.23	76,79,85,86	0
23	SUC	O	4146	23/23	0.73	0.23	68,70,73,76	0
17	8PE	C	4010	47/47	0.81	0.16	39,50,59,60	0
17	8PE	N	4110	47/47	0.82	0.16	43,51,65,67	0
13	6PH	L	4113	40/40	0.86	0.14	51,55,67,68	0
21	CN3	D	4031	55/55	0.86	0.18	48,62,70,71	0
13	6PH	A	4013	40/40	0.89	0.13	48,55,61,61	0
21	CN3	N	4131	55/55	0.90	0.16	39,58,66,69	0
18	9PE	N	4111	40/40	0.91	0.13	39,47,62,66	0
15	HEM	W	4026	43/43	0.92	0.15	46,50,54,55	0
18	9PE	C	4011	40/40	0.93	0.13	39,46,70,72	0
20	7PH	D	4014	38/38	0.94	0.16	43,46,62,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
14	UMQ	A	4021	34/34	0.94	0.11	32,36,55,56	0
20	7PH	O	4114	38/38	0.94	0.15	40,44,52,52	0
14	UMQ	L	4121	34/34	0.94	0.10	33,35,57,58	0
16	SMA	C	4005	37/37	0.95	0.11	22,24,31,34	0
16	SMA	N	4025	37/37	0.95	0.11	21,24,30,33	0
15	HEM	D	4003	43/43	0.97	0.12	23,29,33,34	0
15	HEM	O	4023	43/43	0.98	0.09	25,28,30,33	0
15	HEM	N	4021	43/43	0.98	0.08	16,20,25,27	0
15	HEM	N	4022	43/43	0.98	0.10	15,18,26,28	0
22	FES	P	4024	4/4	0.99	0.09	28,29,31,32	0
22	FES	E	4004	4/4	0.99	0.08	27,27,28,31	0
15	HEM	C	4001	43/43	0.99	0.09	16,21,26,30	0
15	HEM	C	4002	43/43	0.99	0.08	17,20,24,28	0

6.5 Other polymers ⓘ

There are no such residues in this entry.