



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 07:06 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 validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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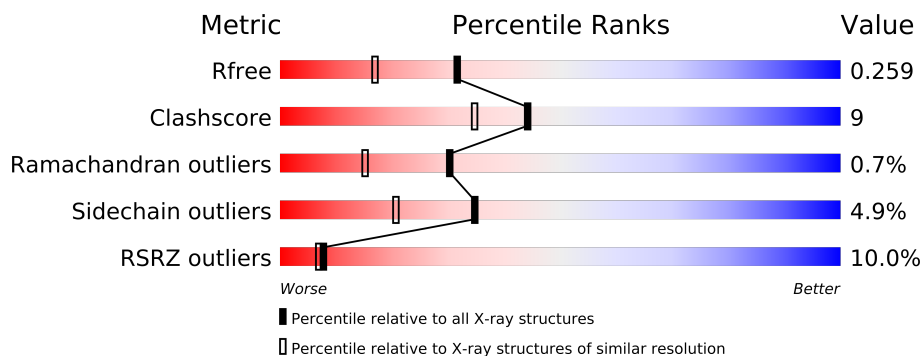
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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))
$R_{free}$	66092	3684 (1.90-1.90)
Clashscore	79885	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (1.90-1.90)
RSRZ outliers	66119	3686 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	431	
1	L	431	
2	B	352	
2	M	352	
3	C	385	
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	

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Mol	Chain	Length	Quality of chain
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 that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
18	8PE	N	4110	-	X
19	9PE	N	4111	-	X
20	CN5	C	4033	-	X

## 2 Entry composition

There are 24 unique types of molecules in this entry. The entry contains 38020 atoms, of which 0 are hydrogen and 0 are deuterium.

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			

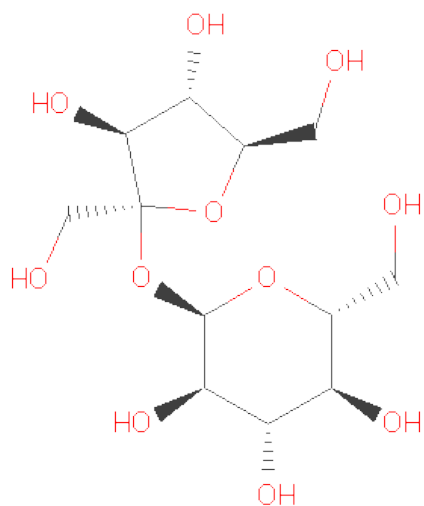
- Molecule 11 is a protein called LIGHT CHAIN (VL) OF FV-FRAGMENT.

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.

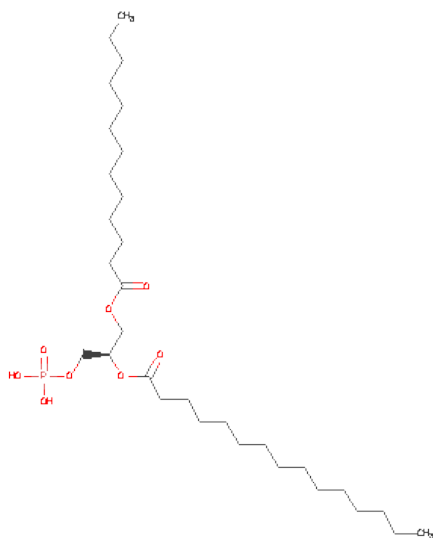
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	W	108	Total	C	N	O	S	0	1	0
			859	542	153	159	5			

- Molecule 13 is SUGAR (SUCROSE) (three-letter code: SUC) (formula: C<sub>12</sub>H<sub>22</sub>O<sub>11</sub>).



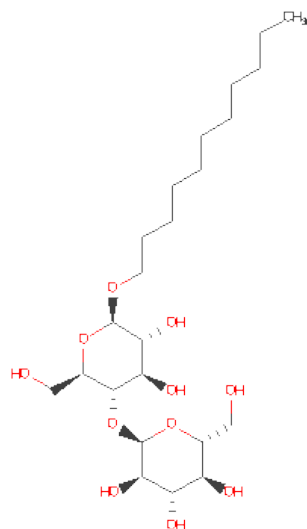
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	O	1	Total	C	O	0	0
			23	12	11		

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



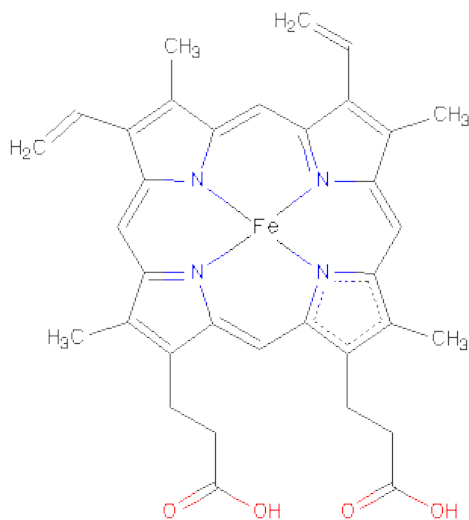
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
14	A	1	40	31	8	1	0	0
14	L	1	40	31	8	1	0	0

- 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	0	0
			34	23	11		
15	L	1	Total	C	O	0	0
			34	23	11		

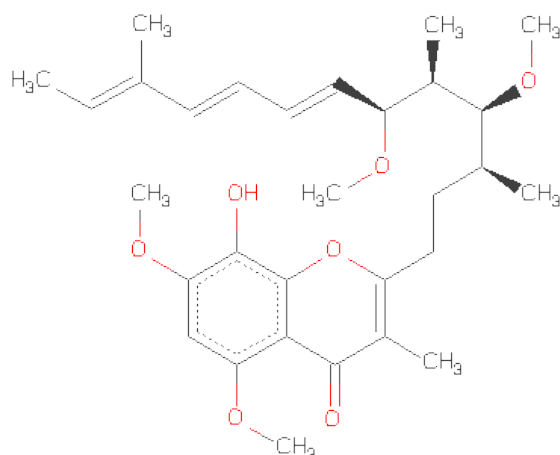
- Molecule 16 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



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

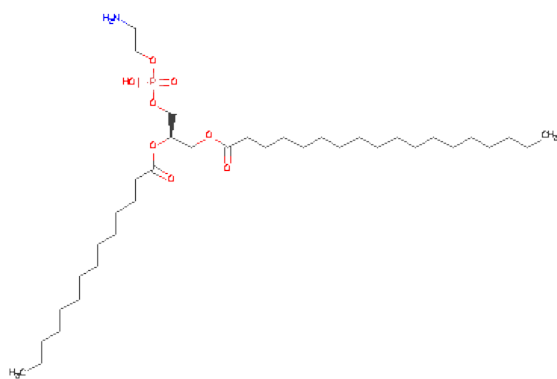
- Molecule 17 is STIGMATELLIN A (three-letter code: SMA) (formula:  $C_{30}H_{42}O_7$ ).





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

- Molecule 18 is (2R)-3-{[(S)-(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-2-(TETRADECANOYLOXY)PROPYLOCTADECANOATE (three-letter code: 8PE) (formula:  $C_{37}H_{74}NO_8P$ ).



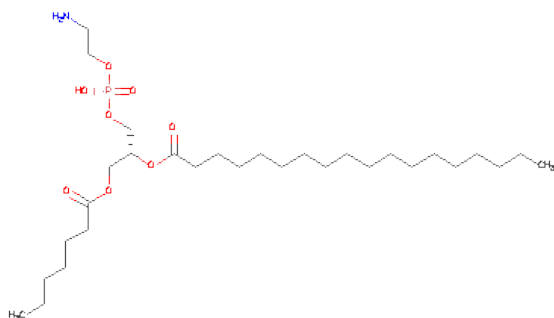
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	C	1	Total	C	N	O	P	0	0
			47	37	1	8	1		

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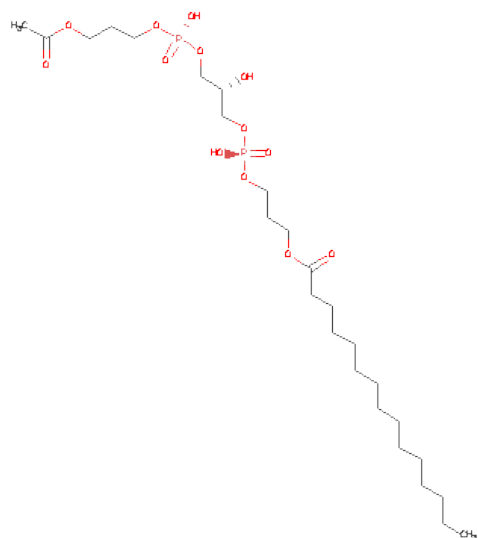
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	N	1	Total	C	N	O	P	0	0
			47	37	1	8	1		

- Molecule 19 is (1R)-2-{[(S)-(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(HEPTANOYLOXY)METHYL]ETHYLOCTADECANOATE (three-letter code: 9PE) (formula: C<sub>30</sub>H<sub>60</sub>NO<sub>8</sub>P).



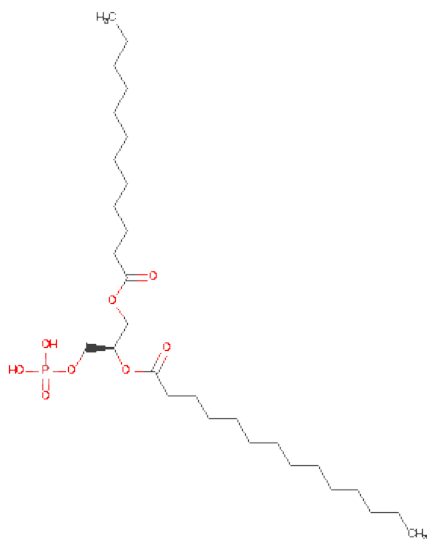
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	C	1	Total	C	N	O	P	0	0
			40	30	1	8	1		
19	N	1	Total	C	N	O	P	0	0
			40	30	1	8	1		

- Molecule 20 is (5S,11R)-5,8,11-TRIHYDROXY-5,11-DIOXIDO-17-OXO-4,6,10,12,16-PENTAOXA-5,11-DIPHOSPHAOCTADEC-1-YLPENTADECANOATE (three-letter code: CN5) (formula: C<sub>26</sub>H<sub>52</sub>O<sub>13</sub>P<sub>2</sub>).



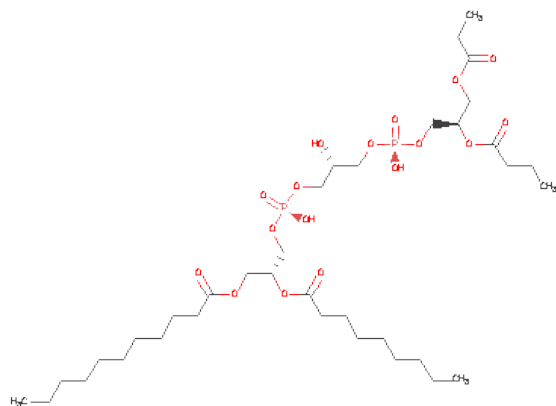
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	C	1	Total	C	O	P	0	0
			41	26	13	2		

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



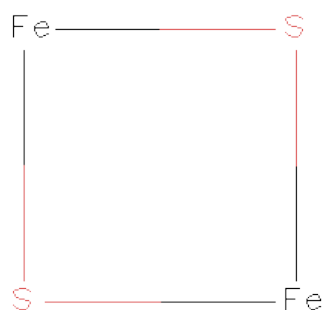
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
21	D	1	Total	C	O	P	0	0
			38	29	8	1		
21	O	1	Total	C	O	P	0	0
			38	29	8	1		

- 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-YLUNDECANOATE (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	0	0
			4	2	2		
23	P	1	Total	Fe	S	0	0
			4	2	2		

- 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		
24	H	31	Total	O	0	0
			31	31		
24	I	11	Total	O	0	0
			11	11		
24	J	15	Total	O	0	0
			15	15		
24	K	7	Total	O	0	0
			7	7		
24	L	170	Total	O	0	0
			170	170		
24	M	101	Total	O	0	0
			101	101		
24	N	170	Total	O	0	0
			170	170		
24	O	173	Total	O	0	0
			173	173		
24	P	66	Total	O	0	0
			66	66		
24	Q	27	Total	O	0	0
			27	27		
24	R	73	Total	O	0	0
			73	73		

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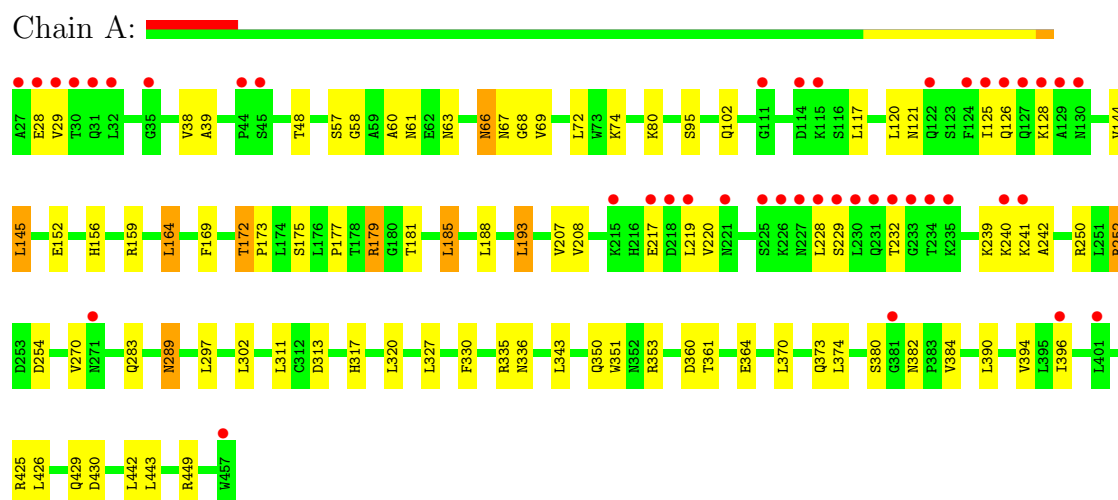
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	S	40	Total 40	O 40	0	0
24	T	12	Total 12	O 12	0	0
24	U	8	Total 8	O 8	0	0
24	V	2	Total 2	O 2	0	0
24	W	20	Total 20	O 20	0	0

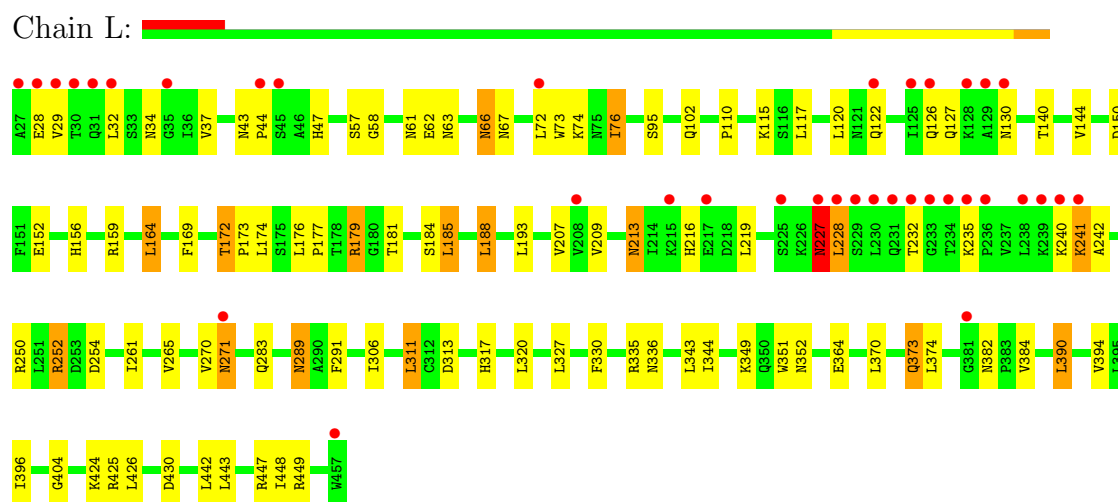
### 3 Residue-property plots

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.

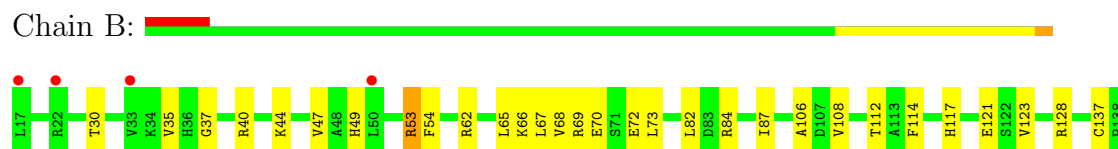
- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial

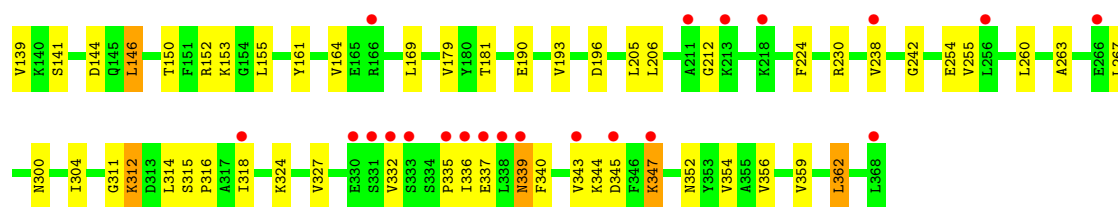


- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial



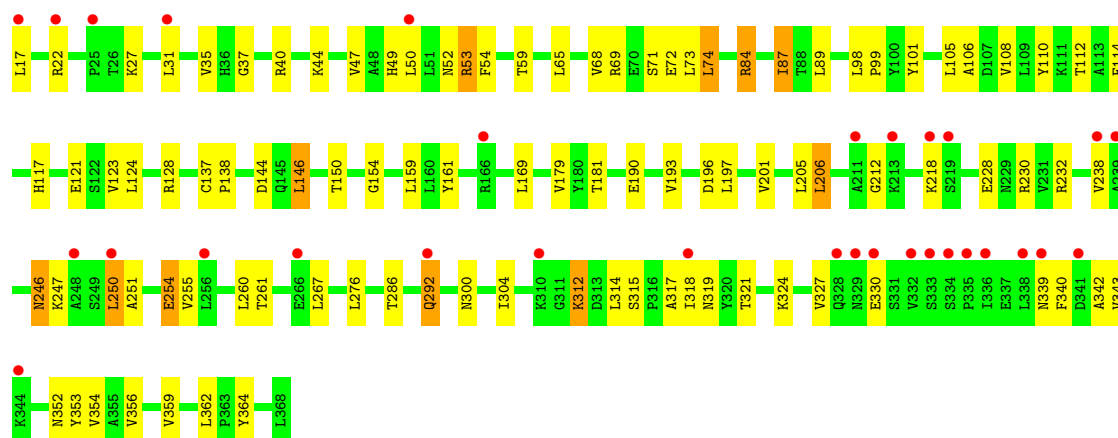
- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial





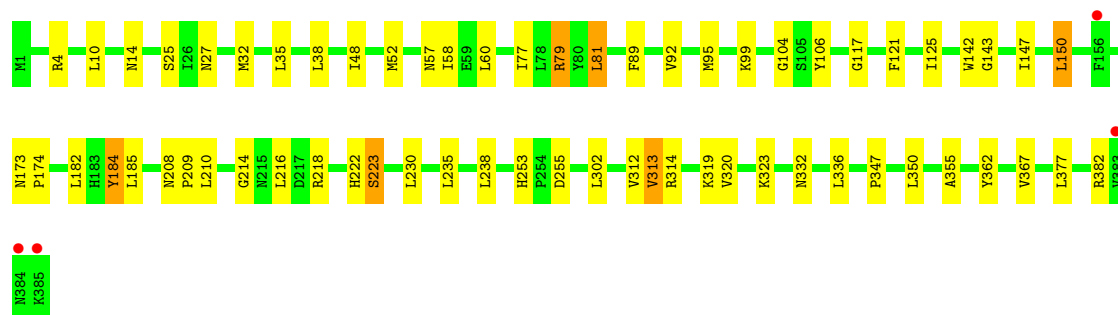
• Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain M:



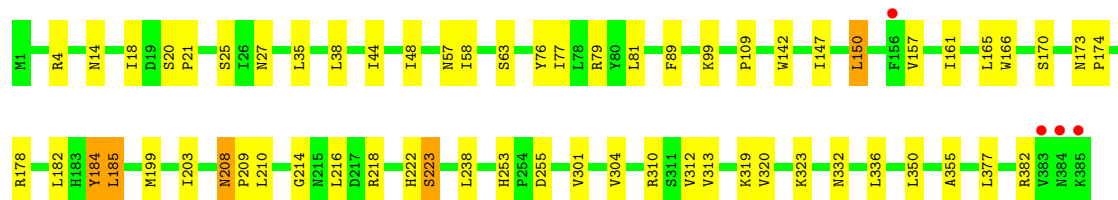
• Molecule 3: CYTOCHROME B

Chain C:



• Molecule 3: CYTOCHROME B

Chain N:



• Molecule 4: Cytochrome c1, heme protein, mitochondrial

Chain D:





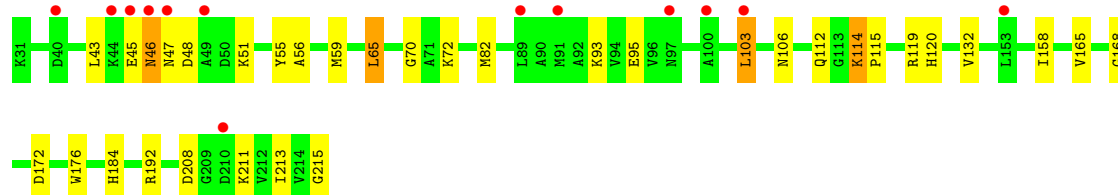
- Molecule 4: Cytochrome c1, heme protein, mitochondrial

Chain O:



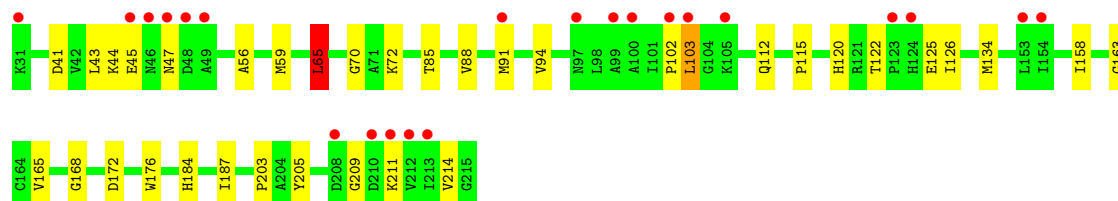
- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain E:



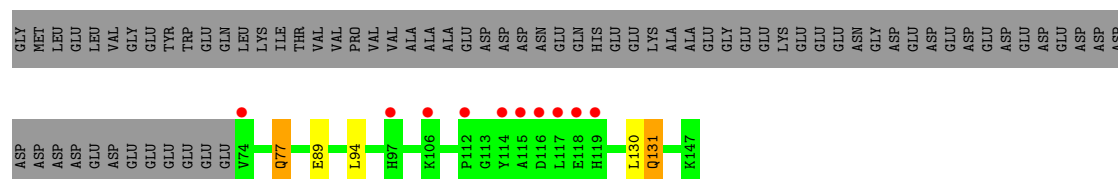
- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain P:



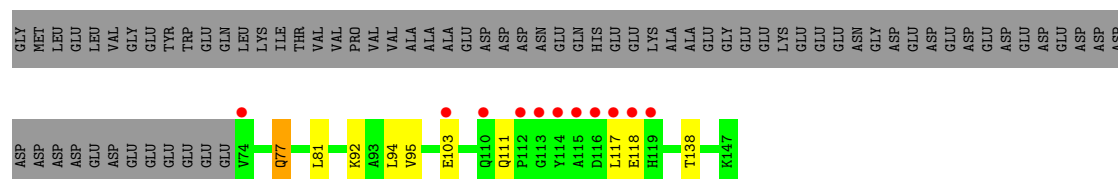
- Molecule 6: Cytochrome b-c1 complex subunit 6

Chain F:



- Molecule 6: Cytochrome b-c1 complex subunit 6

Chain Q:



- Molecule 7: Cytochrome b-c1 complex subunit 7

- Chain R: 

P2	L16	L17	L18	P19	P20	L21	L22	L23	L24	L41	F45	L48	N53	M56	L62	L63	P64	R71	R77	A78	H79	Q80	T84	H85	L88	N91	V100	P101	L120	D121	N122	L123	E124	V125	S126	K127	P128
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- Chain H:

- Chain S: 

32, 35, 36, 37, 38, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 60, 61, 62, 63, 64, 65, 66, 67, 68, 69, 70, 71, 72, 73, 74, 75, 76, 77, 78, 79, 80, 81, 82, 83, 84, 85, 86, 87, 88, 89, 90, 91, 92, 93, 94, 95, 96, 97, 98, 99, 100

- Chain I:

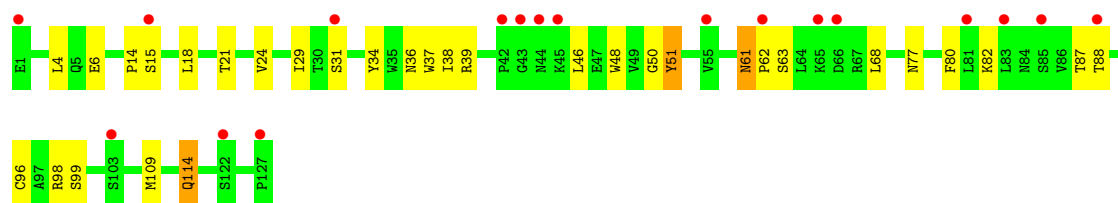
- Chain T: 

- Chain J:

The chart displays the distribution of 100 amino acids across four categories: Aromatic (green), Polar (yellow), Non-polar (orange), and Charged (red). The chart is divided into two rows. The top row contains 48 amino acids, and the bottom row contains 52 amino acids. Each amino acid is represented by a colored bar with its three-letter code and a red dot indicating its category. The categories are: Aromatic (green), Polar (yellow), Non-polar (orange), and Charged (red).

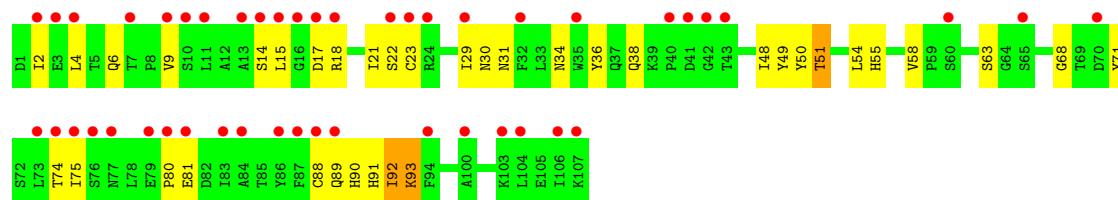
Amino Acid	Category
Trp	Aromatic
Tyr	Polar
Phe	Aromatic
His	Polar
Pro	Non-polar
Gly	Polar
Ala	Non-polar
Val	Non-polar
Ile	Non-polar
Leu	Non-polar
Met	Non-polar
Thr	Polar
Ser	Polar
Asn	Polar
Gln	Polar
Asp	Charged
Glut	Charged
Lys	Charged
Arg	Charged
Pro	Non-polar
Gly	Polar
Ala	Non-polar
Val	Non-polar
Ile	Non-polar
Leu	Non-polar
Met	Non-polar
Thr	Polar
Ser	Polar
Asn	Polar
Gln	Polar
Asp	Charged
Glut	Charged
Lys	Charged
Arg	Charged
Pro	Non-polar
Gly	Polar
Ala	Non-polar
Val	Non-polar
Ile	Non-polar
Leu	Non-polar
Met	Non-polar
Thr	Polar
Ser	Polar
Asn	Polar
Gln	Polar
Asp	Charged
Glut	Charged
Lys	Charged
Arg	Charged

- Chain U: 



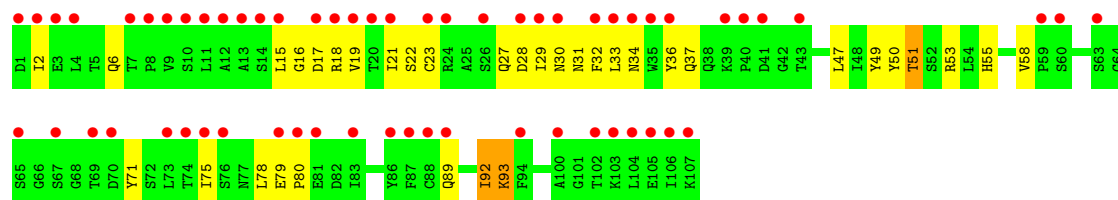
• Molecule 11: LIGHT CHAIN (VL) OF FV-FRAGMENT

Chain K:



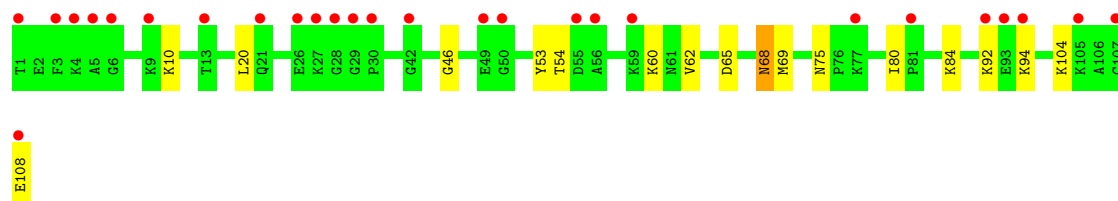
• Molecule 11: LIGHT CHAIN (VL) OF FV-FRAGMENT

Chain V:



• Molecule 12: Cytochrome c iso-1

Chain W:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.33 (at 1.90Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.245 , 0.263 0.243 , 0.259	Depositor DCC
$R_{free}$ test set	33007 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	30.5	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 52.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

## 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(°)	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
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 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

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

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 9.

All (620) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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	Distance(Å)	Clash(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
1:L:283:GLN:NE2	1:L:373:GLN:HE21	1.90	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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

### 5.3.1 Protein backbone ⓘ

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%)	38	23
1	L	429/431 (100%)	406 (95%)	19 (4%)	4 (1%)	25	10
2	B	350/352 (99%)	330 (94%)	15 (4%)	5 (1%)	16	4
2	M	350/352 (99%)	330 (94%)	19 (5%)	1 (0%)	50	37
3	C	383/385 (100%)	370 (97%)	12 (3%)	1 (0%)	50	37
3	N	383/385 (100%)	369 (96%)	13 (3%)	1 (0%)	50	37
4	D	246/248 (99%)	238 (97%)	8 (3%)	0	100	100
4	O	246/248 (99%)	241 (98%)	4 (2%)	1 (0%)	43	29
5	E	183/185 (99%)	173 (94%)	8 (4%)	2 (1%)	21	7
5	P	183/185 (99%)	169 (92%)	10 (6%)	4 (2%)	10	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	21	7
8	S	91/93 (98%)	83 (91%)	7 (8%)	1 (1%)	21	7
9	I	55/65 (85%)	53 (96%)	2 (4%)	0	100	100
9	T	55/65 (85%)	52 (94%)	2 (4%)	1 (2%)	13	3
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%)	5	0
11	V	105/107 (98%)	91 (87%)	11 (10%)	3 (3%)	7	1
12	W	106/108 (98%)	104 (98%)	2 (2%)	0	100	100
All	All	4432/4638 (96%)	4206 (95%)	195 (4%)	31 (1%)	30	15

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
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

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Mol	Chain	Res	Type
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%)	20	8
1	L	370/370 (100%)	340 (92%)	30 (8%)	17	6
2	B	301/301 (100%)	288 (96%)	13 (4%)	40	26
2	M	301/301 (100%)	282 (94%)	19 (6%)	25	12
3	C	338/338 (100%)	318 (94%)	20 (6%)	28	14
3	N	338/338 (100%)	321 (95%)	17 (5%)	34	20
4	D	206/206 (100%)	200 (97%)	6 (3%)	55	44
4	O	206/206 (100%)	202 (98%)	4 (2%)	69	63
5	E	151/151 (100%)	149 (99%)	2 (1%)	80	77
5	P	151/151 (100%)	146 (97%)	5 (3%)	50	37
6	F	67/130 (52%)	62 (92%)	5 (8%)	19	8
6	Q	67/130 (52%)	63 (94%)	4 (6%)	27	13
7	G	110/110 (100%)	105 (96%)	5 (4%)	38	24
7	R	110/110 (100%)	107 (97%)	3 (3%)	57	47
8	H	77/77 (100%)	74 (96%)	3 (4%)	43	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	S	77/77 (100%)	76 (99%)	1 (1%)	80	77
9	I	47/53 (89%)	46 (98%)	1 (2%)	66	59
9	T	47/53 (89%)	45 (96%)	2 (4%)	40	26
10	J	112/112 (100%)	105 (94%)	7 (6%)	25	12
10	U	112/112 (100%)	107 (96%)	5 (4%)	38	24
11	K	93/93 (100%)	88 (95%)	5 (5%)	31	17
11	V	93/93 (100%)	90 (97%)	3 (3%)	51	39
12	W	89/88 (101%)	87 (98%)	2 (2%)	64	57
All	All	3833/3970 (96%)	3644 (95%)	189 (5%)	35	21

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
11	V	91	HIS
12	W	67	ASN
12	W	68	ASN
12	W	75	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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	5.39	2 (18%)	12,14,16	0.96	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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	W	77	M3L	O-C	17.48	1.23	1.11
12	W	77	M3L	CA-C	2.57	1.53	1.48

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	W	77	M3L	CM2-NZ-CM1	-2.01	103.64	109.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	0.97	2 (5%)	44,44,44	1.43	5 (11%)
15	UMQ	A	4021	-	35,35,35	0.89	1 (2%)	46,46,46	1.74	7 (15%)
16	HEM	C	4001	3	49,50,50	1.76	13 (26%)	46,82,82	1.20	3 (6%)
16	HEM	C	4002	3	49,50,50	1.96	14 (28%)	46,82,82	1.17	3 (6%)
17	SMA	C	4005	-	38,38,38	1.13	2 (5%)	50,52,52	2.22	8 (16%)
18	8PE	C	4010	-	46,46,46	0.92	2 (4%)	51,51,51	1.14	3 (5%)
19	9PE	C	4011	-	39,39,39	0.70	0	44,44,44	0.97	2 (4%)
20	CN5	C	4033	-	40,40,40	1.51	7 (17%)	48,48,48	1.68	8 (16%)
16	HEM	D	4003	4	49,50,50	1.98	11 (22%)	46,82,82	1.14	2 (4%)
21	7PH	D	4014	-	37,37,37	0.95	1 (2%)	42,42,42	1.54	10 (23%)
22	CN3	D	4031	-	54,54,54	1.45	9 (16%)	66,66,66	1.44	9 (13%)
23	FES	E	4004	5	0,4,4	0.00	-	0,4,4	0.00	-
14	6PH	L	4113	-	39,39,39	0.98	2 (5%)	44,44,44	1.47	5 (11%)
15	UMQ	L	4121	-	35,35,35	0.92	1 (2%)	46,46,46	1.71	6 (13%)
16	HEM	N	4021	3	49,50,50	1.84	12 (24%)	46,82,82	1.30	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
16	HEM	N	4022	3	49,50,50	1.80	12 (24%)	46,82,82	1.14	3 (6%)
17	SMA	N	4025	-	38,38,38	1.09	2 (5%)	50,52,52	2.29	9 (18%)
18	8PE	N	4110	-	46,46,46	0.97	4 (8%)	51,51,51	1.10	2 (3%)
19	9PE	N	4111	-	39,39,39	0.74	1 (2%)	44,44,44	1.01	2 (4%)
22	CN3	N	4131	-	54,54,54	1.43	10 (18%)	66,66,66	1.41	9 (13%)
16	HEM	O	4023	4	49,50,50	2.08	13 (26%)	46,82,82	1.22	2 (4%)
21	7PH	O	4114	-	37,37,37	0.94	2 (5%)	42,42,42	1.55	10 (23%)
13	SUC	O	4146	-	24,24,24	0.52	0	36,36,36	0.68	1 (2%)
23	FES	P	4024	5	0,4,4	0.00	-	0,4,4	0.00	-
16	HEM	W	4026	12	49,50,50	2.08	16 (32%)	46,82,82	1.35	4 (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
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	-	0/14/114/114	0/0/8/8
16	HEM	C	4002	3	-	0/14/114/114	0/0/8/8
17	SMA	C	4005	-	-	0/33/34/34	0/0/2/2
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	-	0/14/114/114	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	0/0/1/1
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	-	0/14/114/114	0/0/8/8
16	HEM	N	4022	3	-	0/14/114/114	0/0/8/8
17	SMA	N	4025	-	-	0/33/34/34	0/0/2/2
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	-	0/14/114/114	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	0/0/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	HEM	W	4026	12	-	0/14/114/114	0/0/8/8

All (137) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	C	4005	SMA	C4-C4A	5.38	1.48	1.40
17	N	4025	SMA	C4-C4A	5.15	1.48	1.40
16	N	4021	HEM	C3C-C2C	-4.95	1.35	1.43
16	O	4023	HEM	C3B-C2B	-4.95	1.35	1.43
16	D	4003	HEM	C3B-C2B	-4.95	1.35	1.43
16	C	4001	HEM	C3C-C2C	-4.74	1.35	1.43
16	C	4002	HEM	C3D-C2D	-4.70	1.35	1.43
16	N	4022	HEM	C3D-C2D	-4.67	1.35	1.43
16	W	4026	HEM	C3B-C2B	-4.64	1.35	1.43
16	D	4003	HEM	C3C-C2C	-4.63	1.35	1.43
16	N	4022	HEM	C3C-C2C	-4.61	1.35	1.43
16	N	4021	HEM	C3D-C2D	-4.61	1.35	1.43
16	C	4002	HEM	C3B-C2B	-4.56	1.35	1.43
16	O	4023	HEM	C3C-C2C	-4.51	1.35	1.43
16	N	4022	HEM	C3B-C2B	-4.50	1.35	1.43
16	O	4023	HEM	C3B-CAB	4.47	1.54	1.40
16	C	4001	HEM	C3D-C2D	-4.47	1.35	1.43
16	N	4021	HEM	C3B-C2B	-4.47	1.35	1.43
16	W	4026	HEM	C3C-C2C	-4.47	1.36	1.43
16	C	4002	HEM	C2D-C1D	-4.45	1.43	1.44
16	D	4003	HEM	C3D-C2D	-4.45	1.36	1.43
16	C	4002	HEM	C3C-C2C	-4.44	1.36	1.43
16	O	4023	HEM	C3D-C2D	-4.41	1.36	1.43
16	C	4001	HEM	C3B-C2B	-4.40	1.36	1.43
16	O	4023	HEM	CBC-CAC	4.38	1.54	1.28
16	D	4003	HEM	CBC-CAC	4.38	1.54	1.28
16	W	4026	HEM	C3B-CAB	4.32	1.54	1.40
16	O	4023	HEM	CBB-CAB	4.31	1.54	1.28
16	C	4002	HEM	C4A-C3A	4.28	1.45	1.40
16	D	4003	HEM	C3B-CAB	4.27	1.53	1.40
16	W	4026	HEM	CBC-CAC	4.24	1.53	1.28
16	O	4023	HEM	C3C-CAC	4.24	1.53	1.40
22	D	4031	CN3	O31-C3	-4.22	1.35	1.45
16	D	4003	HEM	CBB-CAB	4.22	1.53	1.28
22	N	4131	CN3	O31-C3	-4.21	1.35	1.45
16	W	4026	HEM	C3D-C2D	-4.20	1.36	1.43
16	W	4026	HEM	CBB-CAB	4.12	1.52	1.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	D	4003	HEM	C3C-CAC	3.69	1.52	1.40
16	W	4026	HEM	C3C-CAC	3.65	1.51	1.40
16	N	4022	HEM	C4A-C3A	3.56	1.44	1.40
16	W	4026	HEM	C4A-C3A	3.50	1.44	1.40
22	D	4031	CN3	O21-C2	-3.48	1.37	1.46
21	D	4014	7PH	O31-C3	-3.47	1.37	1.45
16	N	4021	HEM	C4A-C3A	3.45	1.44	1.40
21	O	4114	7PH	O31-C3	-3.36	1.37	1.45
16	C	4002	HEM	CBB-CAB	3.34	1.48	1.28
22	N	4131	CN3	O21-C2	-3.33	1.38	1.46
22	D	4031	CN3	O3'-CA	-3.33	1.31	1.44
15	A	4021	UMQ	C3-C2	-3.32	1.43	1.52
20	C	4033	CN5	P-O14	3.31	1.64	1.51
16	C	4001	HEM	C4A-C3A	3.31	1.44	1.40
15	L	4121	UMQ	C3-C2	-3.30	1.43	1.52
22	N	4131	CN3	O3'-CA	-3.25	1.31	1.44
16	D	4003	HEM	C4A-C3A	3.23	1.44	1.40
20	C	4033	CN5	O3'-CA	-3.20	1.31	1.44
16	N	4022	HEM	CMC-C2C	3.18	1.57	1.47
18	C	4010	8PE	O21-C21	3.17	1.43	1.34
16	O	4023	HEM	C4A-C3A	3.15	1.44	1.40
16	W	4026	HEM	CHA-C4D	3.13	1.40	1.35
18	N	4110	8PE	O21-C21	3.09	1.43	1.34
16	N	4021	HEM	CHB-C1B	3.07	1.40	1.35
16	O	4023	HEM	CHA-C4D	2.97	1.40	1.35
16	W	4026	HEM	FE-NA	2.89	2.04	1.92
16	N	4022	HEM	CBB-CAB	2.87	1.45	1.28
16	C	4001	HEM	CHA-C4D	2.83	1.39	1.35
22	N	4131	CN3	O32-C31	-2.80	1.14	1.22
16	C	4001	HEM	CHB-C1B	2.80	1.39	1.35
16	C	4002	HEM	CBC-CAC	2.73	1.44	1.28
16	C	4001	HEM	CMB-C2B	2.72	1.55	1.47
14	L	4113	6PH	C1-C2	2.71	1.58	1.50
16	C	4001	HEM	CMD-C2D	2.69	1.55	1.47
16	N	4021	HEM	CMD-C2D	2.69	1.55	1.47
20	C	4033	CN5	P'-O2'	2.68	1.61	1.51
16	N	4022	HEM	C3D-C4D	-2.67	1.43	1.44
16	C	4002	HEM	CHB-C1B	2.67	1.39	1.35
16	N	4021	HEM	CMB-C2B	2.66	1.55	1.47
16	W	4026	HEM	CHB-C1B	2.64	1.39	1.35
20	C	4033	CN5	OA-CB	2.63	1.51	1.43
14	L	4113	6PH	C3-C2	2.62	1.58	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	C	4002	HEM	C3D-C4D	-2.61	1.43	1.44
16	N	4021	HEM	CBB-CAB	2.60	1.43	1.28
16	N	4021	HEM	CHD-C4C	2.59	1.41	1.36
22	D	4031	CN3	O32-C31	-2.57	1.15	1.22
16	C	4001	HEM	CBC-CAC	2.55	1.43	1.28
20	C	4033	CN5	P-O11	2.55	1.70	1.59
14	A	4013	6PH	C1-C2	2.54	1.57	1.50
16	O	4023	HEM	C2D-C1D	2.54	1.45	1.44
16	N	4021	HEM	CHA-C4D	2.53	1.39	1.35
16	N	4022	HEM	CBC-CAC	2.53	1.43	1.28
16	C	4002	HEM	CHA-C4D	2.53	1.39	1.35
16	N	4021	HEM	CBC-CAC	2.52	1.43	1.28
16	N	4022	HEM	CHB-C1B	2.51	1.39	1.35
16	N	4021	HEM	CMC-C2C	2.50	1.55	1.47
16	O	4023	HEM	FE-NA	2.48	2.03	1.92
16	C	4002	HEM	CMA-C3A	2.48	1.56	1.51
16	C	4002	HEM	CMC-C2C	2.48	1.55	1.47
22	D	4031	CN3	O11-C1	-2.47	1.34	1.44
16	W	4026	HEM	C3D-C4D	2.47	1.45	1.44
14	A	4013	6PH	C3-C2	2.45	1.57	1.50
16	C	4001	HEM	FE-NA	2.43	2.02	1.92
18	N	4110	8PE	C1-C2	2.40	1.57	1.50
17	N	4025	SMA	C4-C3	2.40	1.48	1.41
22	N	4131	CN3	O21-C21	2.38	1.41	1.34
18	N	4110	8PE	O32-C31	-2.37	1.15	1.22
22	D	4031	CN3	O21-C21	2.34	1.41	1.34
16	C	4001	HEM	CBB-CAB	2.31	1.42	1.28
22	N	4131	CN3	O11-C1	-2.31	1.35	1.44
16	C	4002	HEM	CHC-C1C	2.27	1.40	1.36
16	W	4026	HEM	CMD-C2D	2.27	1.54	1.47
18	C	4010	8PE	O32-C31	-2.25	1.15	1.22
17	C	4005	SMA	C4-C3	2.25	1.47	1.41
16	D	4003	HEM	CHB-C1B	2.19	1.39	1.35
20	C	4033	CN5	P'-O4'	2.19	1.64	1.55
20	C	4033	CN5	CC-CB	2.19	1.60	1.51
18	N	4110	8PE	C3-C2	2.18	1.56	1.50
16	O	4023	HEM	CHD-C4C	2.18	1.40	1.36
22	N	4131	CN3	O41-C3'	-2.17	1.40	1.45
16	C	4001	HEM	CHD-C4C	2.17	1.40	1.36
16	N	4022	HEM	CMD-C2D	2.16	1.54	1.47
22	D	4031	CN3	C1-C2	-2.15	1.44	1.50
16	N	4022	HEM	CMA-C3A	2.14	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	D	4003	HEM	FE-NA	2.14	2.01	1.92
22	D	4031	CN3	CC-CB	2.11	1.60	1.51
16	D	4003	HEM	CHA-C4D	2.11	1.38	1.35
22	D	4031	CN3	OA-CB	2.10	1.50	1.43
16	O	4023	HEM	CHB-C1B	2.10	1.38	1.35
16	W	4026	HEM	CHD-C4C	2.09	1.40	1.36
22	N	4131	CN3	CA-CB	2.08	1.59	1.51
16	W	4026	HEM	CHC-C1C	2.08	1.40	1.36
16	N	4022	HEM	CMB-C2B	2.07	1.53	1.47
22	N	4131	CN3	CC-CB	2.05	1.59	1.51
16	W	4026	HEM	C2D-C1D	2.05	1.45	1.44
16	C	4001	HEM	CMC-C2C	2.04	1.53	1.47
21	O	4114	7PH	O22-C21	-2.04	1.16	1.22
22	N	4131	CN3	OA-CB	2.02	1.49	1.43
16	C	4002	HEM	FE-NA	2.01	2.01	1.92
19	N	4111	9PE	C3-C2	2.00	1.56	1.50

All (117) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	C	4005	SMA	C2-O1-C8A	-11.68	118.26	122.07
17	N	4025	SMA	C2-O1-C8A	-11.68	118.26	122.07
15	A	4021	UMQ	CA-O1'-C1'	-8.34	98.95	113.96
15	L	4121	UMQ	CA-O1'-C1'	-8.07	99.44	113.96
16	W	4026	HEM	C3B-C4B-NB	-6.24	109.53	114.00
17	N	4025	SMA	C9-C2-C3	5.99	127.65	120.42
20	C	4033	CN5	O1'-C1'-C2'	5.76	130.30	109.19
16	N	4021	HEM	C3B-C4B-NB	-5.70	109.92	114.00
16	D	4003	HEM	C3B-C4B-NB	-5.55	110.03	114.00
16	O	4023	HEM	C3B-C4B-NB	-5.46	110.09	114.00
17	C	4005	SMA	C9-C2-C3	5.31	126.83	120.42
22	D	4031	CN3	C2'-O51-C51	-5.23	105.03	117.92
16	C	4001	HEM	C3B-C4B-NB	-5.15	110.31	114.00
16	C	4002	HEM	C3B-C4B-NB	-5.12	110.33	114.00
22	N	4131	CN3	C2'-O51-C51	-4.99	105.60	117.92
14	L	4113	6PH	P-O11-C1	4.89	132.33	118.19
16	N	4022	HEM	C3B-C4B-NB	-4.77	110.59	114.00
20	C	4033	CN5	C3'-C2'-C1'	-4.63	97.68	113.93
14	A	4013	6PH	P-O11-C1	4.59	131.45	118.19
17	C	4005	SMA	C3-C4-C4A	-4.52	114.60	121.65
17	N	4025	SMA	C3-C4-C4A	-4.41	114.77	121.65
14	L	4113	6PH	C3-C2-C1	-4.19	102.31	111.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	4013	6PH	C3-C2-C1	-4.17	102.36	111.86
21	O	4114	7PH	P-O11-C1	4.11	130.09	118.19
21	D	4014	7PH	P-O11-C1	4.03	129.83	118.19
19	N	4111	9PE	C2-O21-C21	-3.83	108.47	117.92
22	N	4131	CN3	C2-O21-C21	-3.82	108.50	117.92
20	C	4033	CN5	O11-C1-C2	-3.73	95.52	109.19
22	D	4031	CN3	C3-C2-C1	-3.70	103.44	111.86
20	C	4033	CN5	P'-O1'-C1'	-3.67	100.98	121.66
22	D	4031	CN3	C2-O21-C21	-3.66	108.89	117.92
19	C	4011	9PE	C2-O21-C21	-3.60	109.04	117.92
17	N	4025	SMA	C9-C10-C11	-3.58	109.61	114.58
18	C	4010	8PE	C3-C2-C1	3.56	119.99	111.86
22	N	4131	CN3	C3-C2-C1	-3.55	103.77	111.86
18	C	4010	8PE	C2-O21-C21	-3.50	109.29	117.92
21	D	4014	7PH	C38-C37-C36	-3.43	96.04	114.61
21	O	4114	7PH	C38-C37-C36	-3.40	96.23	114.61
18	N	4110	8PE	C2-O21-C21	-3.40	109.54	117.92
21	O	4114	7PH	O12-P-O11	3.30	115.75	106.65
15	L	4121	UMQ	O1'-CA-CB	3.28	122.69	109.87
21	D	4014	7PH	O12-P-O11	3.27	115.68	106.65
18	N	4110	8PE	C3-C2-C1	3.19	119.14	111.86
14	A	4013	6PH	O11-P-O12	3.17	116.01	106.71
14	L	4113	6PH	O11-P-O12	3.13	115.89	106.71
21	D	4014	7PH	C3-C2-C1	-3.12	104.74	111.86
22	D	4031	CN3	C3'-C2'-C1'	-3.12	104.75	111.86
17	N	4025	SMA	O1-C2-C9	-3.10	108.84	110.58
15	A	4021	UMQ	O1'-CA-CB	3.08	121.89	109.87
14	L	4113	6PH	O13-P-O11	3.06	115.10	106.65
17	C	4005	SMA	C9-C10-C11	-3.01	110.41	114.58
21	O	4114	7PH	C3-C2-C1	-3.00	105.03	111.86
16	O	4023	HEM	C2D-C1D-ND	-2.95	109.44	112.93
14	A	4013	6PH	O13-P-O11	2.91	114.67	106.65
21	D	4014	7PH	O13-P-O11	2.82	114.42	106.65
21	O	4114	7PH	O13-P-O11	2.79	114.36	106.65
16	N	4021	HEM	CBA-CAA-C2A	-2.79	107.77	112.69
16	W	4026	HEM	C2D-C1D-ND	-2.78	109.65	112.93
15	L	4121	UMQ	O1'-C1'-C2'	2.78	111.71	108.18
16	C	4001	HEM	C2D-C1D-ND	-2.72	109.71	112.93
17	N	4025	SMA	C4-C3-C2	2.71	120.84	116.97
15	A	4021	UMQ	O1'-C1'-C2'	2.70	111.61	108.18
17	C	4005	SMA	C4-C3-C2	2.69	120.81	116.97
16	D	4003	HEM	C2D-C1D-ND	-2.69	109.75	112.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	O	4114	7PH	O31-C3-C2	-2.68	101.79	108.83
16	N	4022	HEM	C2D-C1D-ND	-2.65	109.80	112.93
13	O	4146	SUC	C4-C3-C2	-2.65	105.92	110.82
16	N	4021	HEM	C2D-C1D-ND	-2.62	109.83	112.93
16	C	4002	HEM	C2D-C1D-ND	-2.59	109.87	112.93
16	N	4021	HEM	CAD-C3D-C4D	2.59	129.19	124.53
15	A	4021	UMQ	O1-C1-O5	-2.58	104.27	110.69
22	N	4131	CN3	C3'-C2'-C1'	-2.56	106.02	111.86
14	L	4113	6PH	O14-P-O11	-2.49	99.78	106.65
21	D	4014	7PH	O31-C3-C2	-2.48	102.32	108.83
22	D	4031	CN3	P-O13-CC	2.47	139.82	122.03
15	L	4121	UMQ	C3'-C4'-C5'	-2.44	105.37	110.85
16	C	4001	HEM	CAD-C3D-C4D	2.44	128.91	124.53
22	N	4131	CN3	P-O13-CC	2.38	139.12	122.03
21	D	4014	7PH	O11-P-O14	-2.37	99.76	106.71
15	A	4021	UMQ	CD-CC-CB	-2.37	101.79	114.61
16	W	4026	HEM	CBA-CAA-C2A	-2.37	108.52	112.69
17	C	4005	SMA	O1-C2-C3	2.35	123.87	120.92
15	A	4021	UMQ	C3'-C4'-C5'	-2.34	105.59	110.85
20	C	4033	CN5	C3-C2-C1	-2.33	105.76	113.93
20	C	4033	CN5	C33-C32-C31	2.32	122.59	113.51
17	N	4025	SMA	C3M-C3-C4	-2.31	117.25	120.37
22	D	4031	CN3	O3'-CA-CB	-2.31	101.39	108.62
14	A	4013	6PH	O14-P-O11	-2.30	100.29	106.65
19	N	4111	9PE	O13-P-O11	2.30	111.23	104.68
17	C	4005	SMA	O1-C2-C9	-2.29	109.30	110.58
15	L	4121	UMQ	CD-CC-CB	-2.28	102.29	114.61
21	O	4114	7PH	O31-C31-C32	-2.26	104.84	111.94
16	C	4002	HEM	CMC-C2C-C3C	2.25	131.46	126.16
21	O	4114	7PH	O11-P-O14	-2.24	100.14	106.71
22	N	4131	CN3	O4'-P'-O3'	2.22	119.69	108.51
22	N	4131	CN3	P-O11-C1	-2.21	106.11	122.03
16	N	4022	HEM	CMC-C2C-C3C	2.21	131.36	126.16
15	L	4121	UMQ	O1-C1-O5	-2.21	105.19	110.69
19	C	4011	9PE	O13-P-O11	2.20	110.96	104.68
21	D	4014	7PH	O31-C31-C32	-2.19	105.04	111.94
22	D	4031	CN3	P-O11-C1	-2.17	106.39	122.03
22	N	4131	CN3	O3'-CA-CB	-2.17	101.83	108.62
21	O	4114	7PH	O12-P-O14	-2.16	103.39	110.44
21	D	4014	7PH	O12-P-O14	-2.14	103.43	110.44
22	N	4131	CN3	O11-C1-C2	2.14	121.28	106.02
20	C	4033	CN5	P-O13-CC	2.14	137.44	122.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	W	4026	HEM	CAD-C3D-C4D	2.13	128.36	124.53
18	C	4010	8PE	O31-C3-C2	-2.12	103.27	108.83
17	N	4025	SMA	O8-C8-C7	2.11	124.07	119.35
20	C	4033	CN5	C3-O31-C31	-2.10	111.12	117.02
21	D	4014	7PH	O31-C31-O32	2.09	129.15	123.43
21	O	4114	7PH	O31-C31-O32	2.09	129.15	123.43
17	N	4025	SMA	O1-C2-C3	2.06	123.50	120.92
15	A	4021	UMQ	C1-O5-C5	-2.05	109.74	113.73
22	D	4031	CN3	O4'-P'-O3'	2.04	118.79	108.51
17	C	4005	SMA	C3M-C3-C4	-2.04	117.62	120.37
22	D	4031	CN3	O11-C1-C2	2.00	120.25	106.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	431/431 (100%)	0.50	43 (9%) 8 7	26, 44, 98, 114	0
1	L	431/431 (100%)	0.44	37 (8%) 11 10	25, 42, 90, 113	0
2	B	352/352 (100%)	0.56	25 (7%) 16 15	30, 47, 73, 114	0
2	M	352/352 (100%)	0.53	31 (8%) 10 9	32, 45, 72, 109	0
3	C	385/385 (100%)	-0.13	4 (1%) 79 81	18, 27, 38, 91	0
3	N	385/385 (100%)	-0.17	4 (1%) 79 81	19, 26, 37, 88	0
4	D	248/248 (100%)	0.03	7 (2%) 50 51	25, 35, 57, 83	0
4	O	248/248 (100%)	-0.02	7 (2%) 50 51	24, 33, 55, 86	0
5	E	185/185 (100%)	0.45	13 (7%) 16 16	24, 40, 69, 94	0
5	P	185/185 (100%)	0.62	22 (11%) 5 4	24, 41, 80, 93	0
6	F	74/146 (50%)	0.80	10 (13%) 4 3	34, 46, 90, 96	0
6	Q	74/146 (50%)	0.75	11 (14%) 3 3	32, 45, 87, 90	0
7	G	126/126 (100%)	0.01	6 (4%) 29 30	26, 37, 60, 78	0
7	R	126/126 (100%)	0.03	6 (4%) 29 30	23, 34, 62, 80	0
8	H	93/93 (100%)	1.72	26 (27%) 1 1	24, 45, 128, 131	0
8	S	93/93 (100%)	1.22	18 (19%) 2 1	22, 43, 113, 119	0
9	I	57/65 (87%)	0.76	6 (10%) 7 6	34, 42, 83, 100	0
9	T	57/65 (87%)	0.71	6 (10%) 7 6	32, 40, 84, 96	0
10	J	127/127 (100%)	0.86	15 (11%) 5 4	40, 57, 71, 80	0
10	U	127/127 (100%)	1.04	18 (14%) 3 3	42, 59, 73, 82	0
11	K	107/107 (100%)	2.09	46 (42%) 1 0	51, 81, 114, 116	0
11	V	107/107 (100%)	2.61	60 (56%) 0 0	60, 92, 120, 122	0
12	W	108/108 (100%)	1.33	27 (25%) 1 1	46, 62, 87, 99	0
All	All	4478/4638 (96%)	0.50	448 (10%) 8 7	18, 41, 90, 131	0

All (448) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
8	H	46	PHE	17.6
2	B	338	LEU	16.4
1	L	230	LEU	16.2
9	T	58	ALA	12.5
9	I	57	ALA	12.1
1	A	27	ALA	11.2
8	H	42	HIS	10.9
8	H	49	PHE	10.8
1	A	228	LEU	10.2
8	S	49	PHE	9.7
2	B	336	ILE	9.6
12	W	1	THR	9.5
8	H	41	PHE	9.5
1	A	230	LEU	9.3
8	H	45	VAL	9.2
9	I	58	ALA	9.2
2	B	332	VAL	9.0
8	S	40	ILE	9.0
11	V	15	LEU	8.8
3	C	384	ASN	8.6
9	T	57	ALA	8.2
8	H	44	ALA	8.0
8	S	46	PHE	8.0
3	N	384	ASN	7.9
11	V	106	ILE	7.8
2	M	336	ILE	7.5
8	S	94	VAL	7.5
8	H	40	ILE	7.4
8	S	41	PHE	7.4
8	H	39	GLY	7.3
11	V	79	GLU	7.3
8	H	94	VAL	7.2
2	M	338	LEU	7.2
1	A	129	ALA	7.1
11	K	106	ILE	7.1
6	Q	119	HIS	7.0
11	V	29	ILE	7.0
3	C	383	VAL	6.9
8	H	52	PHE	6.8
2	M	330	GLU	6.7
8	H	43	ASN	6.7
1	A	128	LYS	6.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
8	H	51	ARG	6.7
8	S	38	GLN	6.7
1	A	232	THR	6.6
6	F	119	HIS	6.6
11	K	9	VAL	6.6
1	L	27	ALA	6.6
5	E	47	ASN	6.5
11	V	14	SER	6.5
8	S	39	GLY	6.4
9	I	2	SER	6.4
3	N	385	LYS	6.4
8	H	47	ASN	6.3
1	L	227	ASN	6.2
8	H	37	LEU	6.2
5	E	46	ASN	6.2
4	O	308	ARG	6.1
11	K	16	GLY	6.1
1	A	234	THR	6.1
3	C	385	LYS	6.1
11	K	11	LEU	6.1
11	K	42	GLY	6.0
12	W	9	LYS	6.0
1	L	229	SER	6.0
11	K	107	LYS	5.9
2	M	332	VAL	5.9
4	D	308	ARG	5.9
8	S	44	ALA	5.9
8	S	42	HIS	5.9
1	A	215	LYS	5.7
5	P	100	ALA	5.7
7	R	127	LYS	5.7
5	P	46	ASN	5.6
6	Q	118	GLU	5.5
11	K	80	PRO	5.5
1	A	231	GLN	5.4
11	K	79	GLU	5.4
6	F	117	LEU	5.4
11	V	24	ARG	5.4
11	V	80	PRO	5.3
11	V	107	LYS	5.3
4	O	309	LYS	5.3
6	F	118	GLU	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	227	ASN	5.2
5	E	103	LEU	5.2
5	P	211	LYS	5.1
1	A	229	SER	5.0
5	P	47	ASN	5.0
6	F	115	ALA	4.9
1	L	234	THR	4.9
11	V	70	ASP	4.9
10	U	45	LYS	4.8
8	H	38	GLN	4.8
12	W	55	ASP	4.8
2	B	211	ALA	4.8
5	P	45	GLU	4.8
10	U	66	ASP	4.7
10	U	65	LYS	4.7
10	U	55	VAL	4.7
11	K	14	SER	4.6
7	G	127	LYS	4.6
11	K	75	ILE	4.6
5	E	45	GLU	4.6
4	O	210	PRO	4.5
11	V	100	ALA	4.5
1	L	128	LYS	4.5
11	V	103	LYS	4.5
2	B	337	GLU	4.5
10	J	42	PRO	4.5
5	P	213	ILE	4.5
9	I	56	ILE	4.5
1	L	231	GLN	4.5
2	M	333	SER	4.5
2	M	339	ASN	4.5
1	L	28	GLU	4.4
1	L	125	ILE	4.4
1	L	129	ALA	4.4
5	E	49	ALA	4.4
11	V	7	THR	4.4
11	V	3	GLU	4.4
8	S	37	LEU	4.4
1	A	28	GLU	4.4
8	S	52	PHE	4.3
3	N	383	VAL	4.3
8	H	48	SER	4.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
11	K	40	PRO	4.3
2	M	329	ASN	4.3
1	L	29	VAL	4.2
12	W	108	GLU	4.2
1	A	130	ASN	4.2
10	U	42	PRO	4.2
4	D	309	LYS	4.2
11	V	18	ARG	4.2
11	V	33	LEU	4.2
8	S	43	ASN	4.2
1	A	127	GLN	4.1
5	E	210	ASP	4.1
11	K	17	ASP	4.1
11	V	83	ILE	4.1
11	K	24	ARG	4.1
10	U	43	GLY	4.0
6	F	116	ASP	4.0
11	V	65	SER	4.0
4	D	210	PRO	4.0
6	F	112	PRO	4.0
2	M	344	LYS	4.0
6	Q	112	PRO	4.0
11	V	4	LEU	4.0
8	S	45	VAL	3.9
11	K	15	LEU	3.9
11	V	105	GLU	3.9
2	B	218	LYS	3.9
12	W	28	GLY	3.9
1	A	271	ASN	3.9
1	A	381	GLY	3.9
1	L	238	LEU	3.9
11	V	11	LEU	3.9
9	T	55	ARG	3.9
11	K	43	THR	3.9
9	T	2	SER	3.9
10	J	45	LYS	3.8
2	M	211	ALA	3.7
1	A	44	PRO	3.7
10	J	127	PRO	3.7
2	M	218	LYS	3.7
11	K	10	SER	3.7
11	V	75	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
6	Q	116	ASP	3.7
11	V	12	ALA	3.7
2	M	166	ARG	3.6
11	V	35	TRP	3.6
2	M	318	ILE	3.6
6	Q	115	ALA	3.6
3	N	156	PHE	3.6
12	W	94	LYS	3.5
5	P	91	MET	3.5
1	L	130	ASN	3.5
1	L	457	TRP	3.5
1	L	44	PRO	3.5
4	D	211	GLY	3.5
8	H	53	LYS	3.5
8	H	4	PRO	3.5
11	K	65	SER	3.5
11	V	86	TYR	3.4
5	E	153	LEU	3.4
12	W	27	LYS	3.4
11	V	60	SER	3.4
5	P	210	ASP	3.4
8	S	86	ARG	3.4
2	M	341	ASP	3.4
12	W	49	GLU	3.4
1	A	225	SER	3.4
1	A	29	VAL	3.4
5	P	49	ALA	3.4
10	U	127	PRO	3.4
1	L	31	GLN	3.4
5	E	100	ALA	3.4
11	V	41	ASP	3.4
1	A	35	GLY	3.3
5	E	89	LEU	3.3
11	K	94	PHE	3.3
2	B	266	GLU	3.3
12	W	50	GLY	3.3
11	V	8	PRO	3.3
6	F	74	VAL	3.3
1	A	233	GLY	3.3
12	W	42	GLY	3.3
1	L	217	GLU	3.3
10	U	44	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
10	J	65	LYS	3.2
11	V	10	SER	3.2
1	L	32	LEU	3.2
1	L	235	LYS	3.2
1	A	32	LEU	3.2
2	B	22	ARG	3.2
1	A	124	PHE	3.2
9	T	26	PHE	3.2
11	V	69	THR	3.2
1	A	31	GLN	3.2
2	B	339	ASN	3.2
5	P	153	LEU	3.2
1	L	233	GLY	3.2
2	B	331	SER	3.2
10	U	62	PRO	3.2
1	L	271	ASN	3.2
11	V	30	ASN	3.1
11	V	17	ASP	3.1
5	P	208	ASP	3.1
11	K	23	CYS	3.1
11	K	7	THR	3.1
11	K	29	ILE	3.1
11	V	34	ASN	3.1
1	L	215	LYS	3.1
11	V	9	VAL	3.1
10	U	83	LEU	3.1
11	K	86	TYR	3.1
11	K	100	ALA	3.1
2	B	213	LYS	3.1
6	F	106	LYS	3.1
7	G	23	LYS	3.1
8	H	7	LYS	3.0
11	V	43	THR	3.0
11	K	41	ASP	3.0
12	W	26	GLU	3.0
1	L	232	THR	3.0
8	S	2	GLY	3.0
1	A	241	LYS	3.0
2	B	335	PRO	3.0
1	A	457	TRP	3.0
1	L	126	GLN	3.0
5	P	97	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
10	U	15	SER	2.9
11	K	104	LEU	2.9
10	J	43	GLY	2.9
1	L	240	LYS	2.9
1	A	30	THR	2.9
2	B	166	ARG	2.9
11	V	88	CYS	2.9
1	A	126	GLN	2.9
1	L	239	LYS	2.9
11	K	74	THR	2.9
12	W	59	LYS	2.9
11	K	77	ASN	2.9
2	B	330	GLU	2.9
3	C	156	PHE	2.9
11	K	70	ASP	2.9
12	W	77	M3L	2.9
11	V	23	CYS	2.9
12	W	107	CYS	2.9
1	L	225	SER	2.9
8	H	68	TYR	2.9
2	B	368	LEU	2.9
10	U	31	SER	2.8
8	H	50	ARG	2.8
1	A	240	LYS	2.8
11	K	73	LEU	2.8
8	H	56	PHE	2.8
11	V	73	LEU	2.8
11	V	26	SER	2.8
11	V	94	PHE	2.8
12	W	4	LYS	2.8
11	V	104	LEU	2.8
1	L	35	GLY	2.7
2	B	347	LYS	2.7
11	K	3	GLU	2.7
11	V	20	THR	2.7
11	K	103	LYS	2.7
11	V	81	GLU	2.7
11	V	76	SER	2.7
8	H	86	ARG	2.7
1	L	236	PRO	2.7
7	R	23	LYS	2.7
11	V	32	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
11	V	89	GLN	2.7
6	Q	103	GLU	2.7
11	V	74	THR	2.7
11	V	21	ILE	2.7
12	W	30	PRO	2.7
11	V	36	TYR	2.6
11	V	67	SER	2.6
1	A	235	LYS	2.6
11	V	28	ASP	2.6
1	L	208	VAL	2.6
2	M	238	VAL	2.6
6	Q	114	TYR	2.6
2	B	17	LEU	2.6
11	K	88	CYS	2.6
12	W	21[A]	GLN	2.6
1	A	45	SER	2.6
2	M	250	LEU	2.6
1	A	125	ILE	2.6
11	V	59	PRO	2.6
11	V	19	VAL	2.6
2	B	333	SER	2.5
2	B	50	LEU	2.5
6	Q	74	VAL	2.5
10	J	55	VAL	2.5
2	M	266	GLU	2.5
11	V	39	LYS	2.5
10	J	125	ARG	2.5
1	L	228	LEU	2.5
7	R	20	VAL	2.5
7	G	17	LYS	2.5
7	G	90	ARG	2.5
2	B	238	VAL	2.5
10	U	1	GLU	2.5
4	O	307	PRO	2.4
10	J	62	PRO	2.4
5	E	91	MET	2.4
5	P	124	HIS	2.4
4	D	307	PRO	2.4
12	W	92	LYS	2.4
2	M	31	LEU	2.4
10	J	76	LYS	2.4
12	W	105	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	219	LEU	2.4
2	M	248	ALA	2.4
1	A	115	LYS	2.4
4	D	286	TRP	2.4
11	V	2	ILE	2.4
1	A	226	LYS	2.4
8	H	2	GLY	2.4
2	M	328	GLN	2.4
5	P	48	ASP	2.4
9	T	3	PHE	2.4
2	B	318	ILE	2.4
11	K	76	SER	2.4
8	H	87	GLU	2.3
10	J	1	GLU	2.3
8	S	7	LYS	2.3
10	J	3	LYS	2.3
7	G	19	PRO	2.3
12	W	81	PRO	2.3
1	A	122	GLN	2.3
8	S	5	SER	2.3
11	V	63	SER	2.3
1	L	30	THR	2.3
2	M	17	LEU	2.3
2	M	50	LEU	2.3
5	P	99	ALA	2.3
5	E	97	ASN	2.3
12	W	13	THR	2.3
2	M	292	GLN	2.3
6	Q	110	GLN	2.3
2	B	256	LEU	2.3
6	F	114	TYR	2.3
10	U	103	SER	2.3
11	K	81	GLU	2.3
1	A	401	LEU	2.3
7	R	24	LEU	2.3
10	J	66	ASP	2.3
10	U	81	LEU	2.3
10	J	89	GLU	2.3
10	U	88	THR	2.3
9	I	3	PHE	2.3
11	K	87	PHE	2.3
2	B	343	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
2	M	219	SER	2.2
7	R	126	SER	2.2
5	P	123	PRO	2.2
1	L	72	LEU	2.2
11	K	83	ILE	2.2
11	V	102	THR	2.2
11	K	60	SER	2.2
6	F	97	HIS	2.2
1	A	221	ASN	2.2
11	V	1	ASP	2.2
12	W	56	ALA	2.2
1	L	381	GLY	2.2
6	Q	113	GLY	2.2
12	W	3	PHE	2.2
10	U	122	SER	2.2
2	M	25	PRO	2.2
5	P	154	ILE	2.2
7	R	19	PRO	2.2
11	V	87	PHE	2.2
11	K	89	GLN	2.2
1	A	217	GLU	2.1
8	H	67	TRP	2.1
1	A	111	GLY	2.1
10	J	8	GLY	2.1
2	M	335	PRO	2.1
6	Q	117	LEU	2.1
1	L	122	GLN	2.1
2	B	33	VAL	2.1
1	A	114	ASP	2.1
2	B	345	ASP	2.1
11	V	13	ALA	2.1
11	K	2	ILE	2.1
5	E	44	LYS	2.1
1	A	218	ASP	2.1
10	J	81	LEU	2.1
11	K	32	PHE	2.1
8	S	67	TRP	2.1
12	W	29	GLY	2.1
5	P	102	PRO	2.1
11	K	22	SER	2.1
5	P	31	LYS	2.1
11	K	13	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
12	W	5	ALA	2.1
4	O	141	GLN	2.1
7	G	97	GLN	2.1
2	M	334	SER	2.1
5	P	105	LYS	2.1
2	M	256	LEU	2.1
5	P	103	LEU	2.1
5	E	40	ASP	2.1
4	D	209	PRO	2.0
11	V	40	PRO	2.0
2	M	22	ARG	2.0
11	K	18	ARG	2.0
1	A	396	ILE	2.0
4	O	239	GLY	2.0
11	K	4	LEU	2.0
12	W	6	GLY	2.0
1	L	241	LYS	2.0
2	M	310	LYS	2.0
9	I	26	PHE	2.0
2	M	239	ALA	2.0
1	L	45	SER	2.0
4	O	137	GLU	2.0
2	M	213	LYS	2.0
5	P	212	VAL	2.0
12	W	93	GLU	2.0
10	U	85	SER	2.0
11	K	84	ALA	2.0
11	K	35	TRP	2.0

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

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<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q < 0.9
12	M3L	W	77	12/13	0.30	2.22	64,68,72,72	0

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

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<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
20	CN5	C	4033	41/41	0.23	8.04	76,79,85,86	0
18	8PE	N	4110	47/47	0.17	2.59	43,51,65,67	0
19	9PE	N	4111	40/40	0.14	2.38	39,47,62,66	0
21	7PH	D	4014	38/38	0.15	1.85	43,46,62,63	0
19	9PE	C	4011	40/40	0.13	1.73	39,46,70,72	0
21	7PH	O	4114	38/38	0.14	1.72	40,44,52,52	0
22	CN3	N	4131	55/55	0.17	1.03	39,58,66,69	0
14	6PH	L	4113	40/40	0.14	0.99	51,55,67,68	0
14	6PH	A	4013	40/40	0.13	0.81	48,55,61,61	0
16	HEM	D	4003	43/43	0.12	0.76	23,29,33,34	0
13	SUC	O	4146	23/23	0.22	0.66	68,70,73,76	0
22	CN3	D	4031	55/55	0.18	0.54	48,62,70,71	0
18	8PE	C	4010	47/47	0.16	0.43	39,50,59,60	0
17	SMA	N	4025	37/37	0.11	0.34	21,24,30,33	0
16	HEM	N	4022	43/43	0.10	-0.00	15,18,26,28	0
17	SMA	C	4005	37/37	0.10	-0.02	22,24,31,34	0
16	HEM	O	4023	43/43	0.09	-0.24	25,28,30,33	0
16	HEM	W	4026	43/43	0.14	-0.26	46,50,54,55	0
15	UMQ	A	4021	34/34	0.10	-0.32	32,36,55,56	0
16	HEM	C	4001	43/43	0.09	-0.39	16,21,26,30	0
16	HEM	C	4002	43/43	0.08	-0.41	17,20,24,28	0
15	UMQ	L	4121	34/34	0.10	-0.55	33,35,57,58	0
16	HEM	N	4021	43/43	0.08	-0.67	16,20,25,27	0
23	FES	P	4024	4/4	0.09	-0.83	28,29,31,32	0
23	FES	E	4004	4/4	0.08	-1.42	27,27,28,31	0

### 6.5 Other polymers ⓘ

There are no such residues in this entry.