



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 2, 2017 – 08:44 AM EDT

PDB ID : 3TGU
Title : Cytochrome bc1 complex from chicken with pfvs-designed moa inhibitor bound
Authors : Huang, L.-S.; Yang, G.-F.; Berry, E.A.
Deposited on : unknown
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

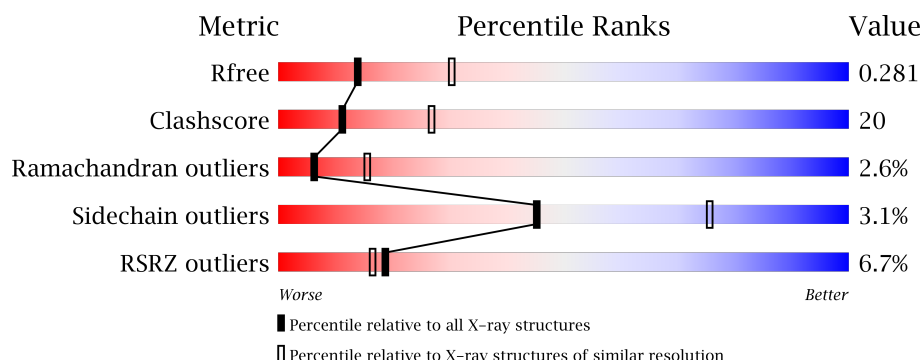
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (2.70-2.70)

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

Mol	Chain	Length	Quality of chain
1	A	446	<div> <div>0.1%</div> <div>67%</div> <div>29%</div> <div>0.1%</div> </div>
1	N	446	<div> <div>2%</div> <div>64%</div> <div>33%</div> <div>1%</div> </div>
2	B	441	<div> <div>3%</div> <div>52%</div> <div>39%</div> <div>5%</div> </div>
2	O	441	<div> <div>5%</div> <div>52%</div> <div>39%</div> <div>4%</div> </div>
3	C	380	<div> <div>3%</div> <div>74%</div> <div>26%</div> <div>0.1%</div> </div>

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Mol	Chain	Length	Quality of chain
3	P	380	
4	D	241	
4	Q	241	
5	E	196	
5	R	196	
6	F	110	
6	S	110	
7	G	81	
7	T	81	
8	H	77	
8	U	77	
9	I	76	
9	V	76	
10	J	61	
10	W	61	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	UNL	A	501	-	-	-	X
11	UNL	N	501	-	-	-	X
14	UQ	C	504	-	-	-	X
14	UQ	P	505	-	-	-	X
15	CDL	C	505	-	-	-	X
15	CDL	Q	502	-	-	-	X
16	PEE	C	507	-	-	-	X
16	PEE	E	502	-	-	-	X
16	PEE	N	502	-	X	-	-
16	PEE	P	507	-	-	-	X
16	PEE	R	502	-	-	-	X
17	GOL	C	508	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	GOL	P	508	-	-	-	X
19	BOG	P	503	-	-	-	X
19	BOG	Q	503	-	-	-	X

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 32733 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Mitochondrial ubiquinol-cytochrome-c reductase complex core protein i.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	443	Total	C	N	O	S	0	0	0
			3442	2157	606	658	21			
1	N	442	Total	C	N	O	S	0	0	0
			3437	2154	605	657	21			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	421	Total	C	N	O	S	0	0	0
			3141	1974	545	613	9			
2	O	422	Total	C	N	O	S	0	0	0
			3147	1977	546	614	10			

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	380	Total	C	N	O	S	0	0	0
			3021	2025	478	505	13			
3	P	379	Total	C	N	O	S	0	0	0
			3012	2019	477	504	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	FME	-	INITIATING METHIONINE	UNP P18946
P	1	FME	-	INITIATING METHIONINE	UNP P18946

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	52	Total	C	N	O	S	0	0	2
			319	190	65	61	3			
9	V	50	Total	C	N	O	S	0	0	2
			311	186	63	59	3			

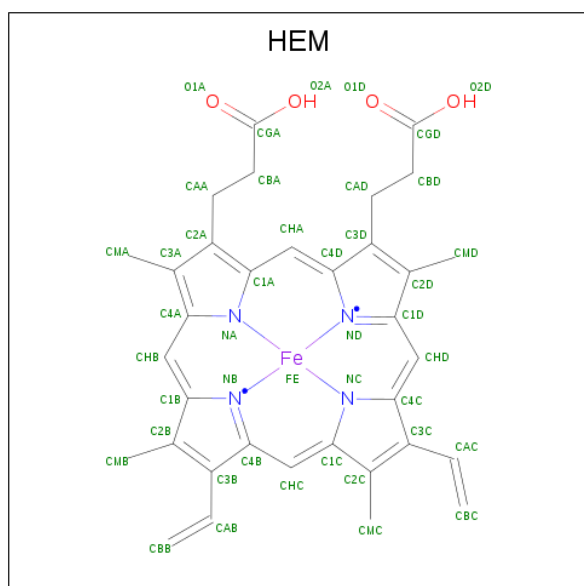
- Molecule 10 is a protein called Mitochondrial ubiquinol-cytochrome c reductase 7.2 kda protein.

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

- Molecule 11 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

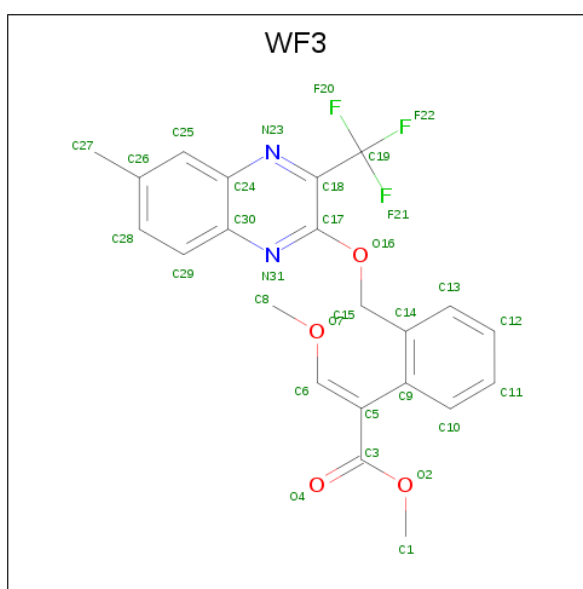
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	1	Total	O	0	0
			1	1		
11	N	1	Total	O	0	0
			1	1		

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



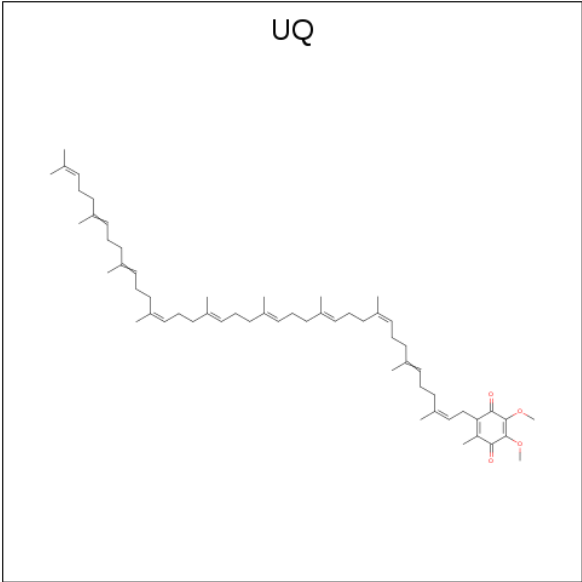
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	
12	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	
12	P	1	Total	C	Fe	N	O	
			43	34	1	4	4	
12	P	1	Total	C	Fe	N	O	
			43	34	1	4	4	

- Molecule 13 is methyl (2E)-3-methoxy-2-[2-([6-methyl-3-(trifluoromethyl)quinoxalin-2-yl]oxy)methyl]phenyl]prop-2-enoate (three-letter code: WF3) (formula: C₂₂H₁₉F₃N₂O₄).



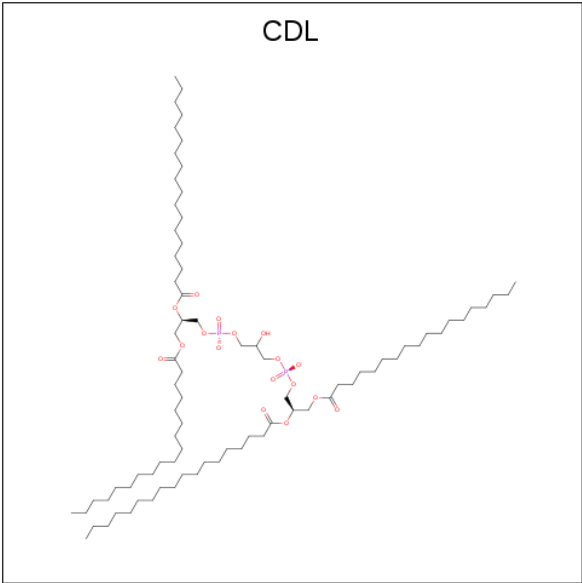
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	C	1	Total	C	F	N	O	
			31	22	3	2	4	
13	P	1	Total	C	F	N	O	
			31	22	3	2	4	

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



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

- Molecule 15 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



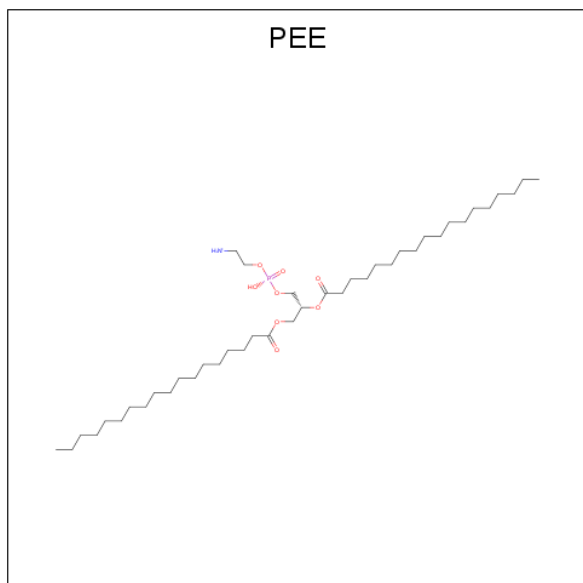
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	C	1	Total	C	O	P	0	0
			42	23	17	2		
15	G	1	Total	C	O	P	0	0
			40	21	17	2		

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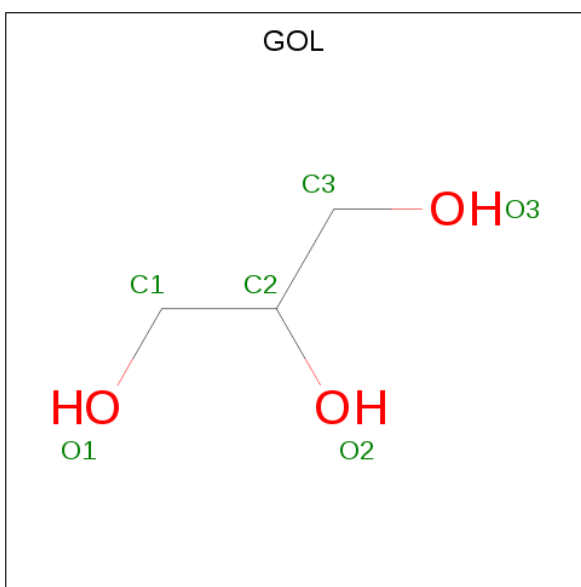
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	P	1	Total	C	O	P	0	0
			40	21	17	2		
15	Q	1	Total	C	O	P	0	0
			42	23	17	2		

- Molecule 16 is 1,2-Dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula: $C_{41}H_{83}NO_8P$).



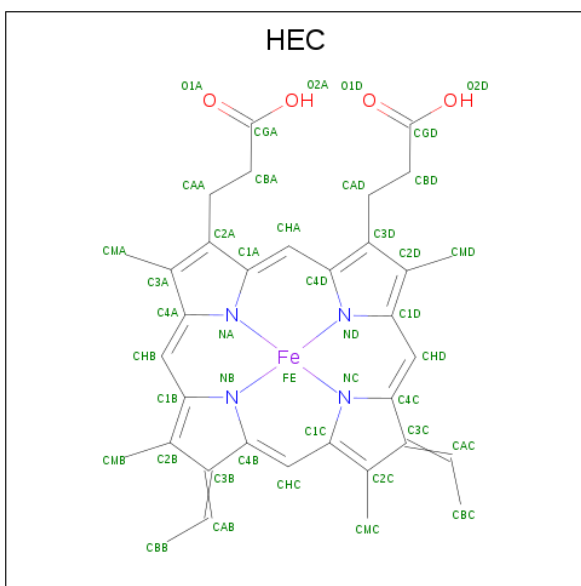
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
16	C	1	Total	C	N	O	P	0	0
			49	39	1	8	1		
16	C	1	Total	C	O	P		0	0
			21	12	8	1			
16	E	1	Total	C	N	O	P	0	0
			50	40	1	8	1		
16	N	1	Total	O	P			0	0
			5	4	1				
16	P	1	Total	C	N	O	P	0	0
			49	39	1	8	1		
16	R	1	Total	C	N	O	P	0	0
			49	39	1	8	1		

- Molecule 17 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



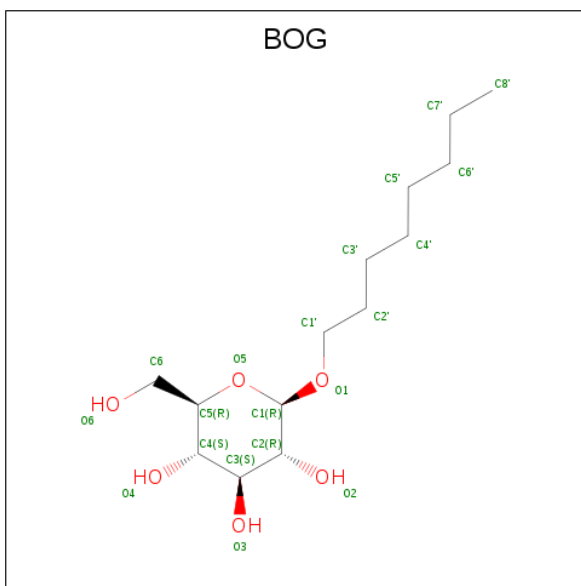
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
17	C	1	Total 6	C 3	O 3	0	0
17	P	1	Total 6	C 3	O 3	0	0

- Molecule 18 is HEME C (three-letter code: HEC) (formula: $\text{C}_{34}\text{H}_{34}\text{FeN}_4\text{O}_4$).



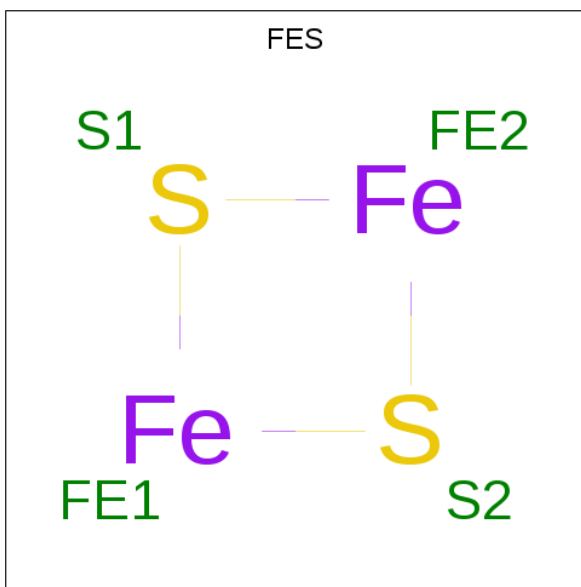
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
18	Q	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 19 is B-OCTYLGLUCOSIDE (three-letter code: BOG) (formula: $C_{14}H_{28}O_6$).



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

- Molecule 20 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



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

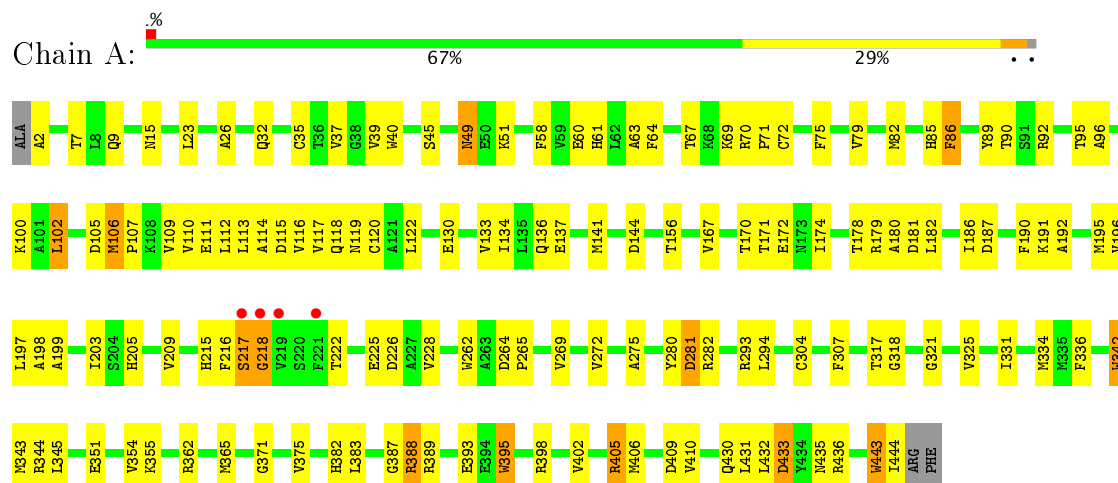
- Molecule 21 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	C	9	Total	O	0	0
			9	9		
21	E	1	Total	O	0	0
			1	1		
21	P	10	Total	O	0	0
			10	10		
21	R	1	Total	O	0	0
			1	1		

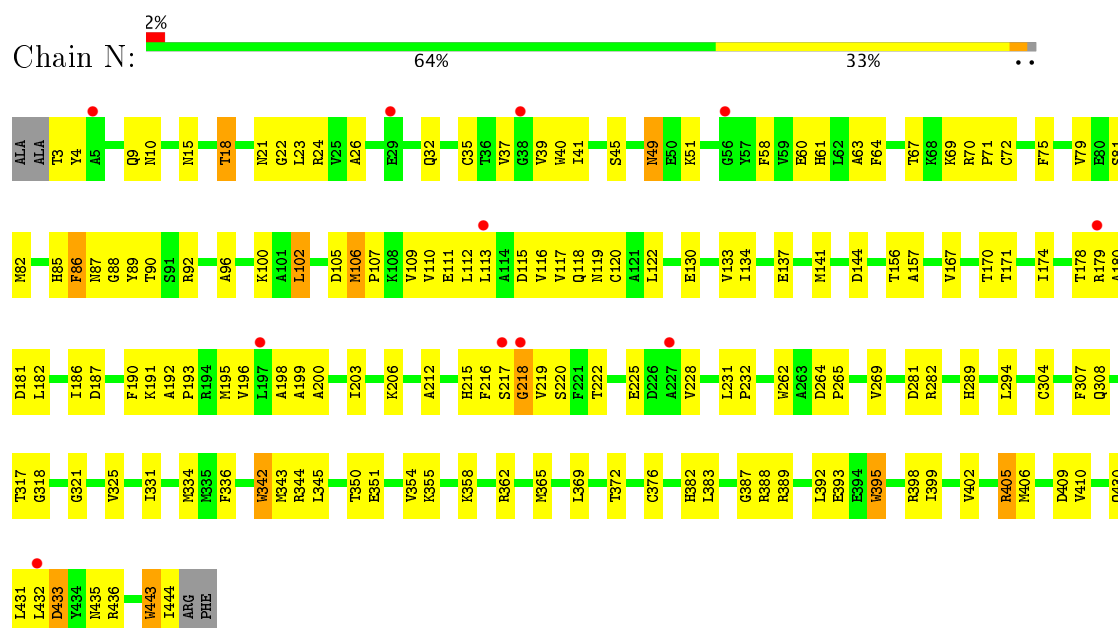
3 Residue-property plots

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

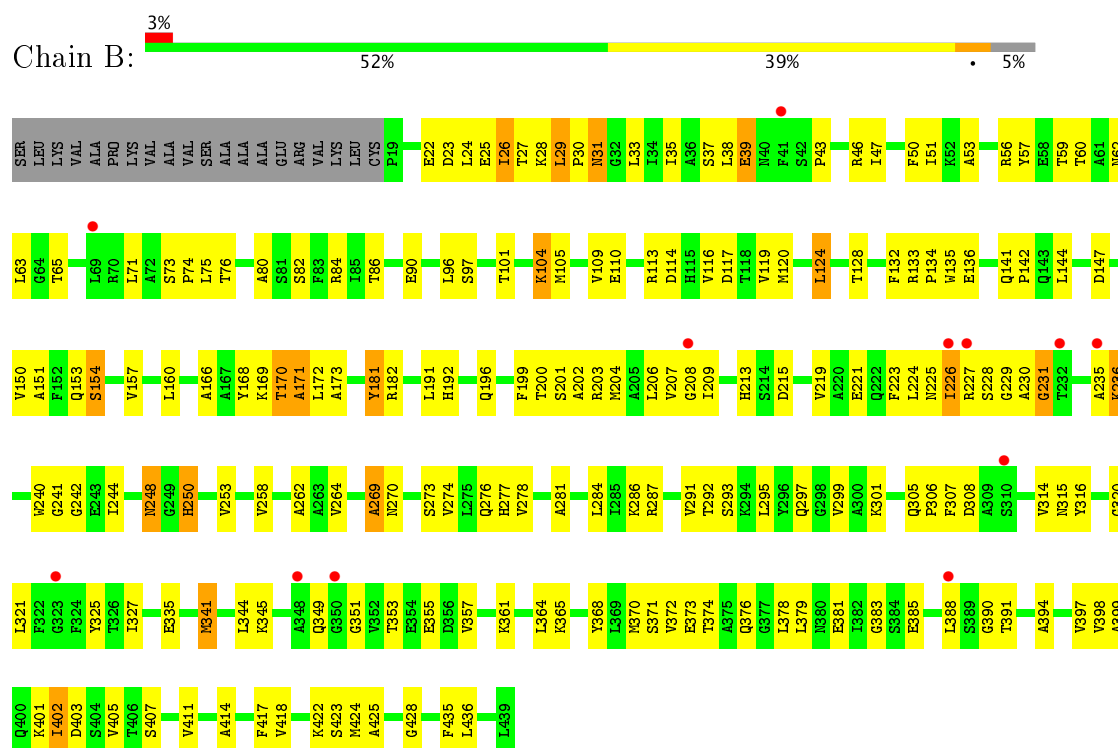
- Molecule 1: Mitochondrial ubiquinol-cytochrome-c reductase complex core protein i



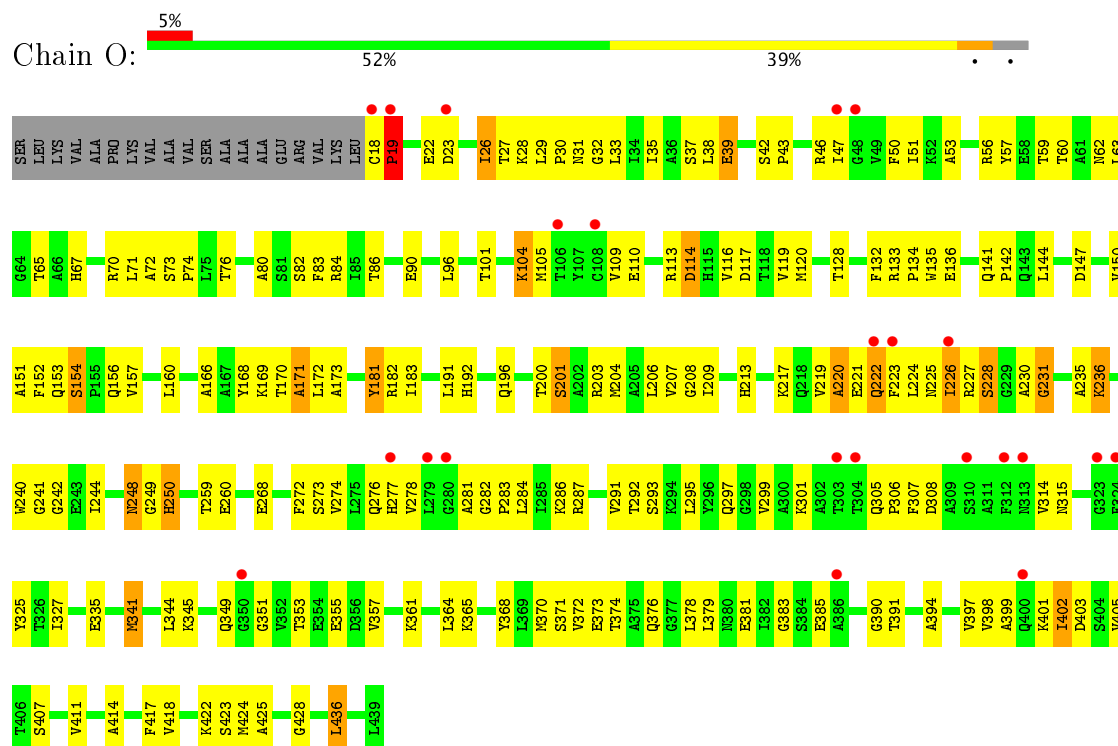
- Molecule 1: Mitochondrial ubiquinol-cytochrome-c reductase complex core protein i



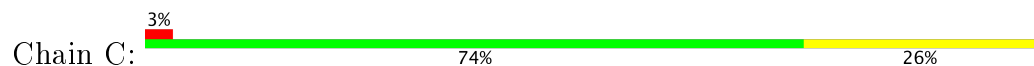
- Molecule 2: Mitochondrial ubiquinol-cytochrome-c reductase complex core protein 2

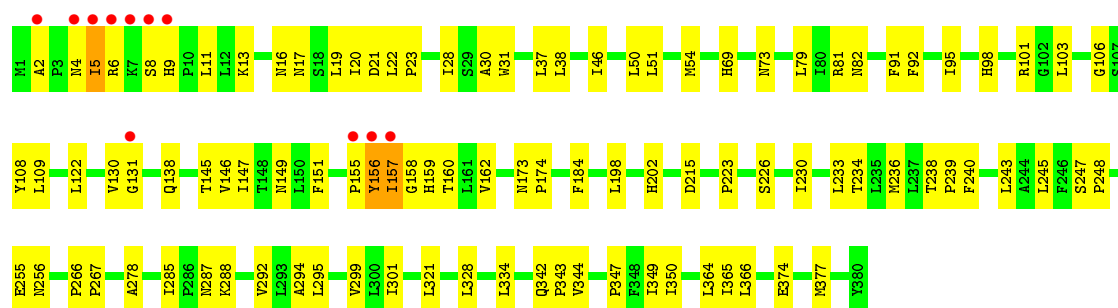


• Molecule 2: Mitochondrial ubiquinol-cytochrome-c reductase complex core protein 2

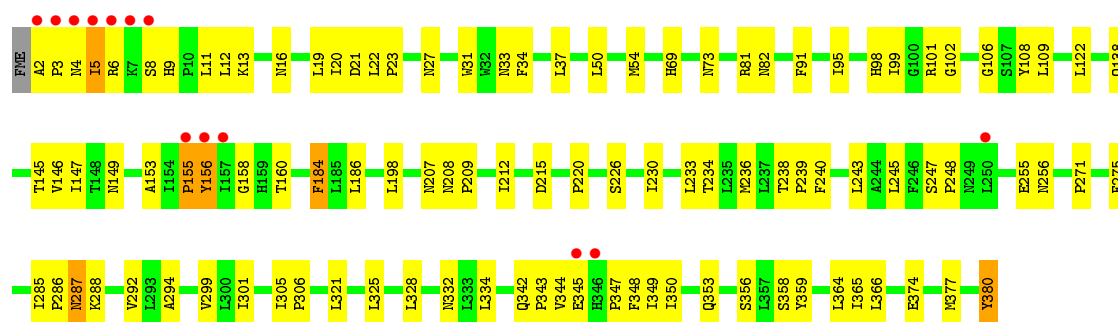


• Molecule 3: Cytochrome b

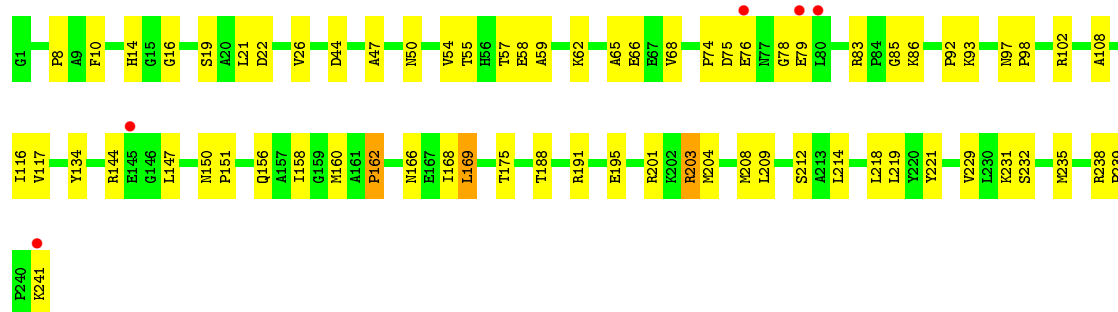




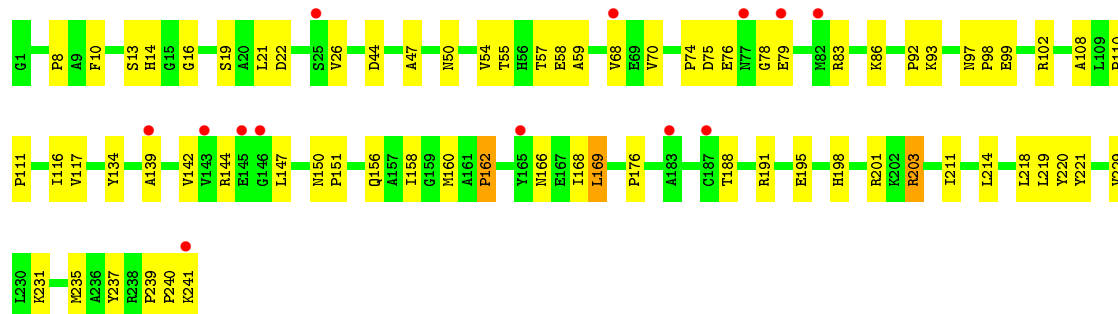
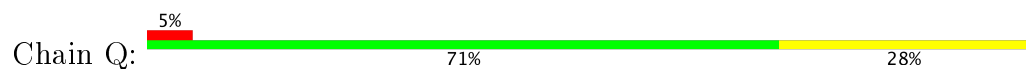
• Molecule 3: Cytochrome b



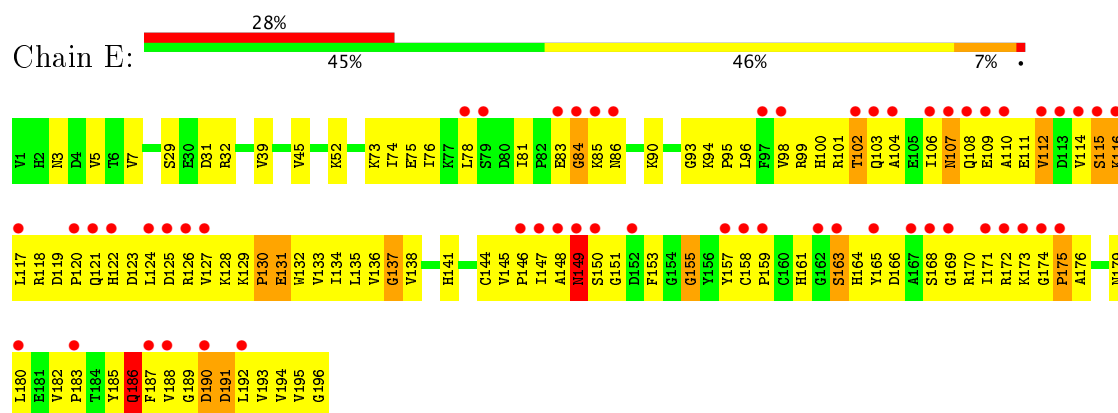
• Molecule 4: Mitochondrial cytochrome c1, heme protein



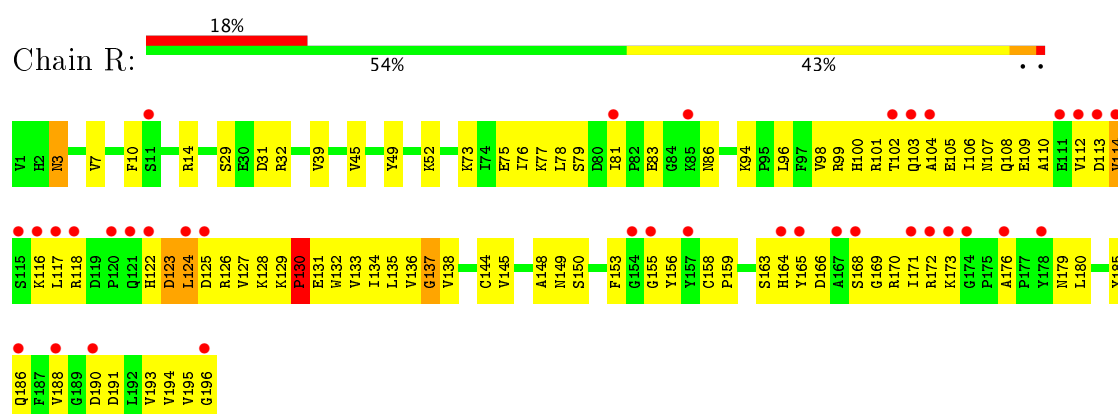
• Molecule 4: Mitochondrial cytochrome c1, heme protein



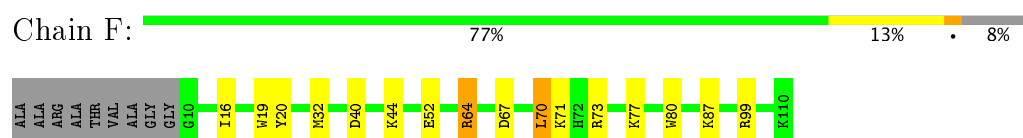
- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial



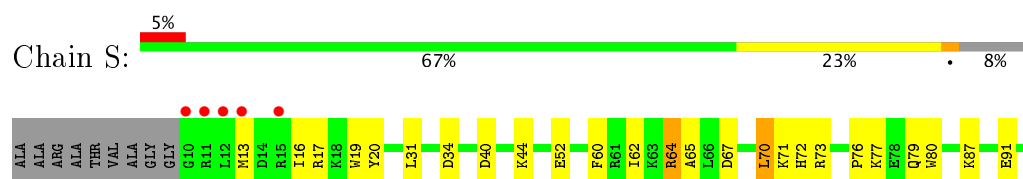
- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial



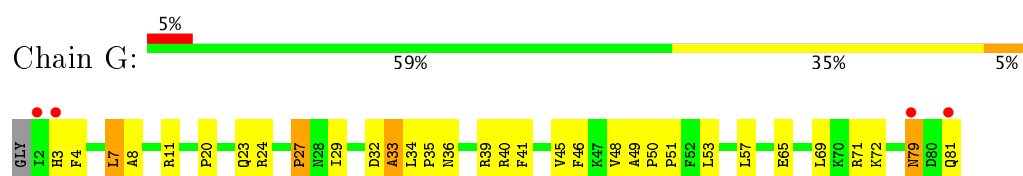
- Molecule 6: Mitochondrial ubiquinol-cytochrome c reductase 14 kda protein



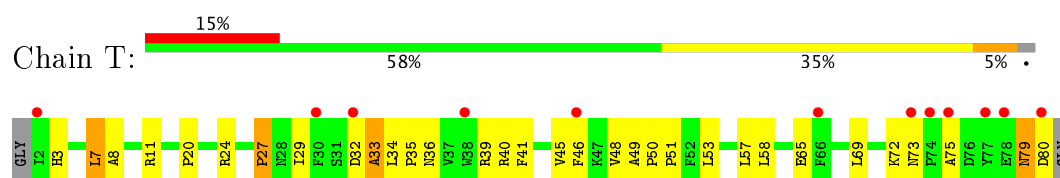
- Molecule 6: Mitochondrial ubiquinol-cytochrome c reductase 14 kda protein



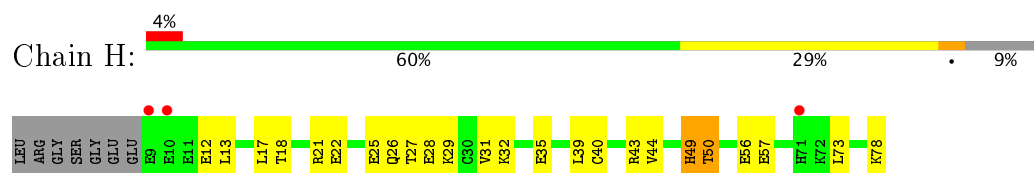
- Molecule 7: Mitochondrial ubiquinol-cytochrome c reductase ubiquinone-binding protein qp-c



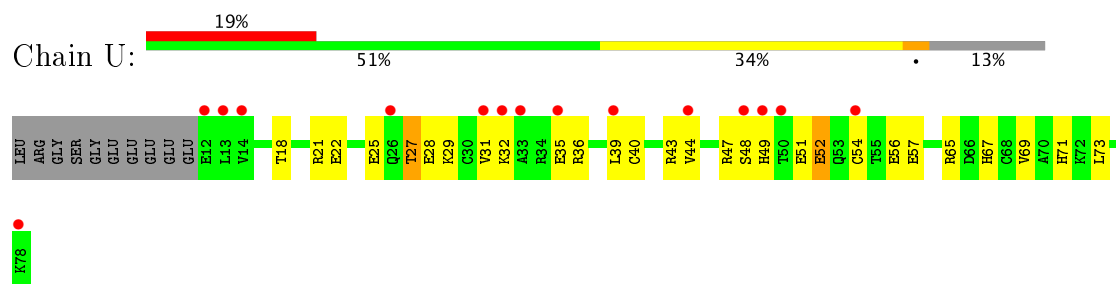
- Molecule 7: Mitochondrial ubiquinol-cytochrome c reductase ubiquinone-binding protein qp-c



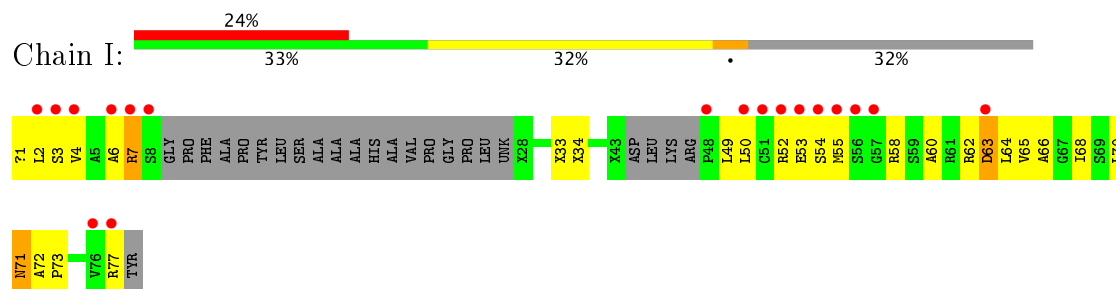
- Molecule 8: Mitochondrial ubiquinol-cytochrome c reductase 11 kda protein, complex iii subunit viii



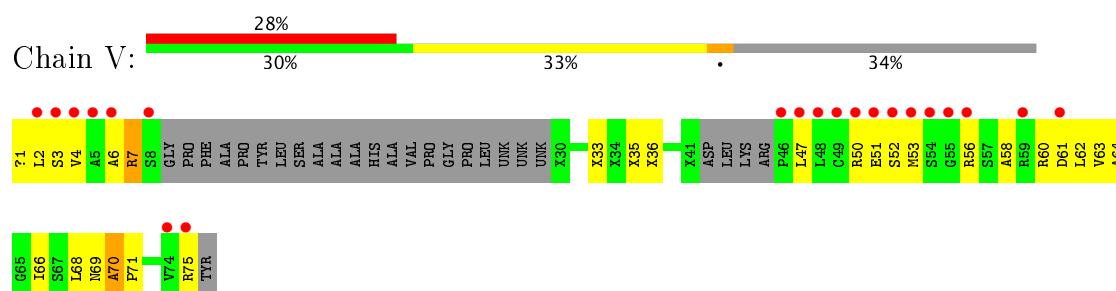
- Molecule 8: Mitochondrial ubiquinol-cytochrome c reductase 11 kda protein, complex iii subunit viii



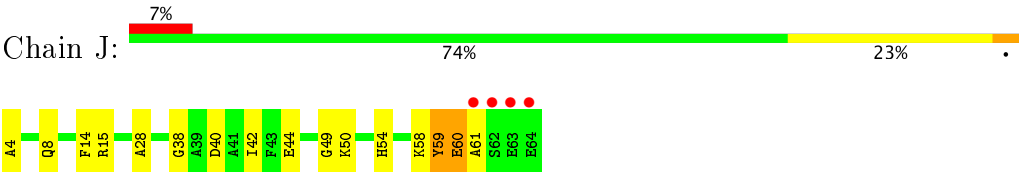
- Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial



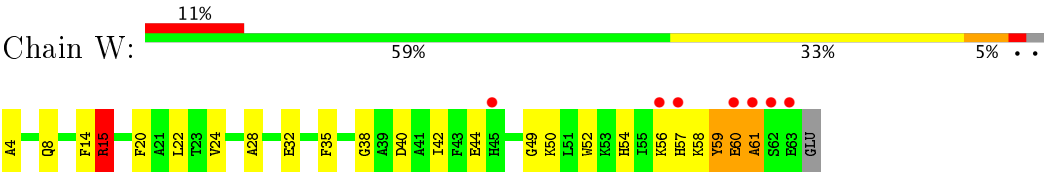
- Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	172.68Å 183.31Å 241.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.98 – 2.70 24.98 – 2.70	Depositor EDS
% Data completeness (in resolution range)	91.1 (24.98-2.70) 91.2 (24.98-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.72Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.258 , 0.289 0.253 , 0.281	Depositor DCC
R_{free} test set	3737 reflections (1.99%)	DCC
Wilson B-factor (Å ²)	60.9	Xtriage
Anisotropy	0.687	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 75.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	32733	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.85% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CDL, UQ, AME, UNL, FES, HEC, WF3, FME, PEE, HEM, BOG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.39	0/3513	0.64	0/4760
1	N	0.40	0/3508	0.63	0/4753
2	B	0.35	0/3196	0.62	0/4334
2	O	0.37	0/3202	0.63	0/4343
3	C	0.45	0/3114	0.65	0/4263
3	P	0.42	0/3114	0.63	0/4263
4	D	0.41	0/1956	0.62	0/2658
4	Q	0.37	0/1956	0.60	0/2658
5	E	0.35	0/1547	0.59	0/2103
5	R	0.35	0/1543	0.60	0/2098
6	F	0.47	0/911	0.65	0/1219
6	S	0.38	0/911	0.60	0/1219
7	G	0.44	0/694	0.65	0/941
7	T	0.41	0/684	0.64	0/929
8	H	0.39	0/582	0.60	0/779
8	U	0.32	0/561	0.58	0/751
9	I	0.36	0/251	0.62	0/336
9	V	0.34	0/251	0.60	0/336
10	J	0.39	0/508	0.59	0/682
10	W	0.41	0/490	0.58	0/660
All	All	0.39	0/32492	0.62	0/44085

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3442	0	3354	119	0
1	N	3437	0	3349	134	0
2	B	3141	0	3142	195	0
2	O	3147	0	3146	213	0
3	C	3021	0	3068	74	0
3	P	3012	0	3058	79	0
4	D	1898	0	1846	58	0
4	Q	1898	0	1846	59	0
5	E	1513	0	1478	108	0
5	R	1509	0	1474	92	0
6	F	891	0	893	16	0
6	S	891	0	893	29	0
7	G	672	0	653	29	0
7	T	662	0	645	33	0
8	H	574	0	548	18	0
8	U	553	0	535	29	0
9	I	319	0	281	43	0
9	V	311	0	283	48	0
10	J	497	0	490	13	0
10	W	479	0	478	22	0
11	A	1	0	0	0	0
11	N	1	0	0	0	0
12	C	86	0	60	5	0
12	P	86	0	60	4	0
13	C	31	0	19	1	0
13	P	31	0	19	1	0
14	C	19	0	17	3	0
14	P	19	0	17	2	0
15	C	42	0	28	1	0
15	G	40	0	24	1	0
15	P	40	0	24	3	0
15	Q	42	0	28	1	0
16	C	70	0	85	2	0
16	E	50	0	77	0	0
16	N	5	0	0	0	0
16	P	49	0	72	2	0
16	R	49	0	71	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	C	6	0	8	0	0
17	P	6	0	8	0	0
18	D	43	0	30	2	0
18	Q	43	0	30	1	0
19	D	33	0	39	0	0
19	P	12	0	11	0	0
19	Q	33	0	39	0	0
20	E	4	0	0	0	0
20	R	4	0	0	0	0
21	C	9	0	0	0	0
21	E	1	0	0	0	0
21	P	10	0	0	2	0
21	R	1	0	0	0	0
All	All	32733	0	32226	1293	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

All (1293) 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:O:76:THR:HG22	2:O:82:SER:H	1.05	1.19
1:N:178:THR:HG22	1:N:180:ALA:H	1.10	1.14
1:A:178:THR:HG22	1:A:180:ALA:H	1.11	1.13
2:B:76:THR:HG22	2:B:82:SER:H	1.12	1.12
1:A:69:LYS:HD2	1:A:70:ARG:HH21	1.12	1.10
8:U:36:ARG:HB3	8:U:36:ARG:HH11	1.18	1.08
1:N:69:LYS:HD2	1:N:70:ARG:HH21	1.17	1.07
1:N:102:LEU:HD12	1:N:102:LEU:H	1.18	1.06
9:V:35:UNK:HG3	9:V:36:UNK:H	1.15	1.05
2:B:22:GLU:HG3	2:B:23:ASP:H	1.20	1.05
9:I:33:UNK:HG3	9:I:34:UNK:H	1.19	1.02
1:A:102:LEU:H	1:A:102:LEU:HD12	1.23	1.02
5:R:83:GLU:HB3	5:R:102:THR:HG22	1.39	1.01
5:E:83:GLU:HB3	5:E:102:THR:HG22	1.44	0.98
4:D:47:ALA:H	4:D:50:ASN:HD22	1.02	0.98
8:U:36:ARG:NH1	8:U:36:ARG:HB3	1.80	0.96
2:O:341:MET:HE2	2:O:341:MET:HA	1.46	0.96
2:O:37:SER:HB3	2:O:213:HIS:ND1	1.80	0.96
2:B:341:MET:HE2	2:B:341:MET:HA	1.49	0.95
4:Q:47:ALA:H	4:Q:50:ASN:HD22	1.00	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:394:ALA:HB3	2:B:397:VAL:HG23	1.51	0.93
2:O:101:THR:HG21	9:V:4:VAL:HG11	1.48	0.93
5:E:116:LYS:H	5:E:116:LYS:HD2	1.33	0.93
2:B:353:THR:HG22	2:B:355:GLU:H	1.33	0.92
2:O:101:THR:HG23	2:O:104:LYS:HE3	1.52	0.91
2:O:353:THR:HG22	2:O:355:GLU:H	1.33	0.90
2:O:157:VAL:HG23	9:V:62:LEU:HD21	1.53	0.90
1:N:206:LYS:H	1:N:206:LYS:HD2	1.37	0.89
4:Q:47:ALA:H	4:Q:50:ASN:ND2	1.71	0.88
2:B:101:THR:HG23	2:B:104:LYS:HE3	1.54	0.88
5:R:78:LEU:HB3	5:R:132:TRP:CZ2	2.09	0.87
2:B:157:VAL:HG23	9:I:64:LEU:HD21	1.55	0.87
2:O:394:ALA:HB3	2:O:397:VAL:HG23	1.53	0.87
1:N:106:MET:HG3	1:N:203:ILE:HD13	1.57	0.86
2:O:76:THR:HG22	2:O:82:SER:N	1.89	0.86
2:B:37:SER:HB3	2:B:213:HIS:ND1	1.91	0.86
5:R:117:LEU:HD21	5:R:172:ARG:NH1	1.91	0.86
2:O:385:GLU:HG2	9:V:2:LEU:HD13	1.58	0.85
2:O:291:VAL:HA	2:O:297:GLN:HE21	1.41	0.84
4:Q:231:LYS:O	6:S:71:LYS:HE3	1.75	0.84
1:A:178:THR:HG22	1:A:180:ALA:N	1.94	0.83
2:B:80:ALA:HA	2:B:84:ARG:HH12	1.44	0.83
2:B:315:ASN:HD22	9:I:7:ARG:HD3	1.43	0.82
6:S:13:MET:HA	6:S:16:ILE:HD12	1.62	0.82
5:E:107:ASN:N	5:E:107:ASN:HD22	1.78	0.82
2:O:27:THR:HG22	2:O:28:LYS:H	1.42	0.82
4:D:57:THR:HG22	4:D:59:ALA:H	1.43	0.82
1:A:106:MET:HG3	1:A:203:ILE:HD13	1.60	0.82
1:A:178:THR:HB	1:A:181:ASP:OD1	1.78	0.82
1:N:178:THR:HG22	1:N:180:ALA:N	1.92	0.82
1:N:39:VAL:HG11	1:N:117:VAL:HG11	1.63	0.81
2:O:96:LEU:HB3	9:V:68:LEU:HD22	1.62	0.81
3:P:301:ILE:HD11	3:P:364:LEU:HD21	1.62	0.81
2:O:221:GLU:HG3	2:O:222:GLN:H	1.45	0.81
8:H:27:THR:HG22	8:H:29:LYS:H	1.45	0.80
4:Q:57:THR:HG22	4:Q:59:ALA:H	1.44	0.80
8:U:27:THR:HG22	8:U:29:LYS:H	1.44	0.80
2:B:76:THR:HG22	2:B:82:SER:N	1.94	0.80
3:P:2:ALA:HB3	3:P:8:SER:HB3	1.64	0.80
1:A:69:LYS:HD2	1:A:70:ARG:NH2	1.95	0.80
2:O:38:LEU:HG	2:O:39:GLU:H	1.47	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:47:ALA:H	4:D:50:ASN:ND2	1.77	0.80
2:O:291:VAL:HA	2:O:297:GLN:NE2	1.96	0.79
1:A:39:VAL:HG11	1:A:117:VAL:HG11	1.65	0.79
2:B:241:GLY:HA2	2:B:423:SER:HB3	1.65	0.79
1:N:196:VAL:HG11	1:N:383:LEU:HD12	1.62	0.79
2:B:291:VAL:HA	2:B:297:GLN:HE21	1.46	0.79
10:W:60:GLU:HG2	10:W:60:GLU:O	1.80	0.78
2:O:381:GLU:OE1	9:V:3:SER:HB2	1.83	0.78
2:B:38:LEU:HG	2:B:39:GLU:H	1.49	0.78
2:O:80:ALA:HA	2:O:84:ARG:HH12	1.48	0.78
2:B:27:THR:HG22	2:B:28:LYS:H	1.48	0.78
3:P:238:THR:HB	3:P:239:PRO:HD3	1.66	0.78
4:D:144:ARG:HG2	4:D:147:LEU:HD12	1.66	0.77
5:E:136:VAL:HG23	5:E:183:PRO:HD3	1.63	0.77
5:E:119:ASP:HB3	5:E:179:ASN:ND2	2.00	0.77
4:D:57:THR:HG22	4:D:59:ALA:N	2.00	0.77
1:N:69:LYS:HD2	1:N:70:ARG:NH2	1.98	0.77
5:R:112:VAL:HG21	5:R:170:ARG:HH22	1.49	0.76
2:B:291:VAL:HA	2:B:297:GLN:NE2	1.99	0.76
2:O:209:ILE:HD13	2:O:378:LEU:HD23	1.67	0.76
5:R:104:ALA:HA	5:R:107:ASN:ND2	2.01	0.76
1:A:443:TRP:CE3	1:A:443:TRP:HA	2.21	0.75
1:N:182:LEU:O	1:N:186:ILE:HG13	1.86	0.75
1:N:85:HIS:CD2	2:O:284:LEU:HD22	2.22	0.75
2:O:62:ASN:O	2:O:65:THR:HG22	1.86	0.75
9:V:3:SER:HB3	9:V:6:ALA:HB3	1.69	0.75
2:O:154:SER:O	2:O:157:VAL:HG12	1.87	0.75
2:O:46:ARG:HG2	2:O:379:LEU:HD22	1.68	0.75
1:A:2:ALA:HB3	2:B:113:ARG:HH21	1.52	0.74
3:C:301:ILE:HD11	3:C:364:LEU:HD21	1.67	0.74
9:I:49:LEU:HD22	9:I:54:SER:O	1.87	0.74
1:N:102:LEU:N	1:N:102:LEU:HD12	2.00	0.74
9:V:47:LEU:HD22	9:V:52:SER:O	1.86	0.74
1:N:178:THR:HB	1:N:181:ASP:OD1	1.85	0.74
1:A:336:PHE:CZ	3:C:4:ASN:HB3	2.22	0.74
2:B:207:VAL:HG21	2:B:383:GLY:HA2	1.68	0.74
1:A:85:HIS:CD2	2:B:284:LEU:HD22	2.23	0.74
1:N:187:ASP:O	1:N:191:LYS:HE3	1.88	0.73
2:B:209:ILE:HD13	2:B:378:LEU:HD23	1.69	0.73
1:N:443:TRP:CE3	1:N:443:TRP:HA	2.22	0.73
2:O:207:VAL:HG21	2:O:383:GLY:HA2	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:315:ASN:HD22	9:V:7:ARG:HD3	1.53	0.73
1:N:206:LYS:N	1:N:206:LYS:HD2	2.04	0.73
2:B:306:PRO:HA	9:I:52:ARG:HG3	1.69	0.73
2:O:361:LYS:O	2:O:365:LYS:HG3	1.89	0.73
2:O:327:ILE:HD11	9:V:56:ARG:O	1.89	0.73
2:O:248:ASN:HD22	2:O:248:ASN:C	1.89	0.73
9:I:3:SER:HB3	9:I:6:ALA:HB3	1.71	0.73
2:B:22:GLU:HG3	2:B:23:ASP:N	2.01	0.72
1:N:18:THR:HG23	1:N:24:ARG:HG3	1.70	0.72
9:V:63:VAL:HB	9:V:75:ARG:HD3	1.70	0.72
4:Q:57:THR:HG22	4:Q:59:ALA:N	2.03	0.72
1:A:187:ASP:O	1:A:191:LYS:HE3	1.88	0.72
3:C:37:LEU:HD21	3:C:233:LEU:HA	1.71	0.72
5:E:171:ILE:HG22	5:E:179:ASN:OD1	1.90	0.72
9:I:64:LEU:HD12	9:I:77:ARG:C	2.10	0.72
6:F:32:MET:HE1	6:F:87:LYS:HG2	1.71	0.72
2:O:181:TYR:CE1	2:O:182:ARG:HG3	2.24	0.72
1:N:102:LEU:CD1	1:N:102:LEU:H	1.97	0.72
5:R:81:ILE:HG22	5:R:100:HIS:HB2	1.72	0.72
2:B:56:ARG:NH1	2:B:172:LEU:HG	2.04	0.72
3:C:238:THR:HB	3:C:239:PRO:HD3	1.71	0.72
2:O:27:THR:HG22	2:O:28:LYS:N	2.03	0.72
1:N:443:TRP:HE3	1:N:443:TRP:HA	1.54	0.72
2:B:46:ARG:HG2	2:B:379:LEU:HD22	1.71	0.72
2:B:62:ASN:O	2:B:65:THR:HG22	1.90	0.72
7:T:24:ARG:HB2	7:T:27:PRO:HB3	1.72	0.72
3:P:101:ARG:C	3:P:101:ARG:HD2	2.11	0.71
10:W:40:ASP:O	10:W:44:GLU:HG3	1.89	0.71
1:A:443:TRP:HE3	1:A:443:TRP:HA	1.55	0.71
9:I:70:LEU:HD23	9:I:71:ASN:HD22	1.55	0.71
5:R:94:LYS:HD3	5:R:138:VAL:HG21	1.72	0.71
2:B:63:LEU:HB2	2:B:182:ARG:HD3	1.70	0.71
1:A:182:LEU:O	1:A:186:ILE:HG13	1.89	0.71
4:D:231:LYS:O	6:F:71:LYS:HE3	1.90	0.71
2:O:221:GLU:HG3	2:O:222:GLN:N	2.05	0.71
2:O:295:LEU:O	2:O:299:VAL:HG23	1.91	0.71
2:O:314:VAL:HG13	9:V:61:ASP:HB3	1.73	0.71
3:P:37:LEU:HD21	3:P:233:LEU:HA	1.71	0.71
2:B:38:LEU:CG	2:B:39:GLU:H	2.04	0.70
2:B:27:THR:HG22	2:B:28:LYS:N	2.06	0.70
2:O:38:LEU:CG	2:O:39:GLU:H	2.05	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:295:LEU:O	2:B:299:VAL:HG23	1.91	0.70
2:B:202:ALA:HB3	2:B:229:GLY:O	1.92	0.70
1:A:102:LEU:N	1:A:102:LEU:HD12	2.02	0.70
5:E:78:LEU:HD12	5:E:190:ASP:O	1.92	0.70
2:O:22:GLU:HG3	2:O:23:ASP:H	1.56	0.70
2:B:150:VAL:O	2:B:153:GLN:HG3	1.91	0.70
4:Q:144:ARG:HG2	4:Q:147:LEU:HD12	1.73	0.70
2:B:399:ALA:O	2:B:402:ILE:HG22	1.92	0.69
5:E:129:LYS:HG3	5:E:187:PHE:CZ	2.27	0.69
2:O:248:ASN:HD21	2:O:250:HIS:HB2	1.57	0.69
9:V:35:UNK:HG3	9:V:36:UNK:N	1.95	0.69
2:O:241:GLY:HA2	2:O:423:SER:HB3	1.72	0.69
15:P:506:CDL:OA4	7:T:40:ARG:HD2	1.92	0.69
2:O:150:VAL:O	2:O:153:GLN:HG3	1.92	0.69
2:B:154:SER:O	2:B:157:VAL:HG12	1.93	0.69
2:O:63:LEU:HB2	2:O:182:ARG:HD3	1.76	0.68
5:R:169:GLY:O	5:R:179:ASN:HB3	1.92	0.68
2:B:31:ASN:N	2:B:31:ASN:HD22	1.91	0.68
2:O:56:ARG:NH1	2:O:172:LEU:HG	2.09	0.68
5:R:109:GLU:OE1	5:R:123:ASP:HB2	1.93	0.68
3:P:342:GLN:HE21	3:P:343:PRO:HD2	1.59	0.68
4:Q:8:PRO:HG2	4:Q:10:PHE:CE1	2.27	0.68
1:A:196:VAL:HG11	1:A:383:LEU:HD12	1.76	0.68
2:O:399:ALA:O	2:O:402:ILE:HG22	1.93	0.68
8:H:28:GLU:HG2	8:H:32:LYS:HE3	1.76	0.67
1:A:186:ILE:HG23	1:A:190:PHE:CD1	2.29	0.67
1:N:336:PHE:CZ	3:P:4:ASN:HB3	2.28	0.67
2:O:26:ILE:HD13	2:O:391:THR:HA	1.76	0.67
2:B:361:LYS:O	2:B:365:LYS:HG3	1.94	0.67
10:J:40:ASP:O	10:J:44:GLU:HG3	1.95	0.67
3:P:22:LEU:HD21	14:P:505:UQ:HM32	1.77	0.67
2:B:248:ASN:HD22	2:B:248:ASN:C	1.98	0.67
1:A:69:LYS:CD	1:A:70:ARG:HH21	1.99	0.67
2:B:357:VAL:HG12	2:B:361:LYS:HE3	1.77	0.67
2:O:43:PRO:O	2:O:113:ARG:HG3	1.95	0.67
3:C:236:MET:O	3:C:239:PRO:HD2	1.94	0.67
8:U:28:GLU:HG2	8:U:32:LYS:HE3	1.77	0.67
18:Q:501:HEC:HMB1	18:Q:501:HEC:HBB3	1.77	0.67
9:V:62:LEU:HD12	9:V:75:ARG:C	2.15	0.67
2:B:101:THR:HG21	9:I:4:VAL:HG11	1.77	0.66
4:D:102:ARG:HA	4:D:108:ALA:O	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:D:501:HEC:HBB3	18:D:501:HEC:HMB1	1.76	0.66
7:G:40:ARG:HD2	15:G:101:CDL:OA4	1.95	0.66
10:J:15:ARG:HH11	10:J:15:ARG:HG2	1.59	0.66
2:O:169:LYS:HG3	2:O:240:TRP:HB2	1.77	0.66
1:A:102:LEU:H	1:A:102:LEU:CD1	2.01	0.66
2:B:181:TYR:CE1	2:B:182:ARG:HG3	2.31	0.66
9:I:49:LEU:HD13	9:I:55:MET:HG2	1.78	0.66
2:B:307:PHE:H	9:I:52:ARG:HG2	1.58	0.66
2:O:46:ARG:NH2	2:O:376:GLN:HG3	2.10	0.66
5:E:84:GLY:N	5:E:102:THR:HG23	2.10	0.66
1:N:170:THR:HG22	1:N:171:THR:N	2.11	0.66
7:T:29:ILE:O	7:T:33:ALA:HB3	1.95	0.66
3:C:377:MET:HE2	6:F:20:TYR:HB2	1.77	0.66
8:H:40:CYS:O	8:H:44:VAL:HG23	1.96	0.66
9:V:35:UNK:CG	9:V:36:UNK:H	2.00	0.66
2:B:169:LYS:O	2:B:170:THR:HG23	1.95	0.66
4:D:26:VAL:HG22	4:D:188:THR:HG22	1.78	0.65
5:E:96:LEU:HD12	5:E:135:LEU:O	1.96	0.65
10:W:15:ARG:HH11	10:W:15:ARG:HG2	1.61	0.65
3:P:9:HIS:O	3:P:13:LYS:HB3	1.95	0.65
1:N:105:ASP:O	1:N:109:VAL:HG23	1.96	0.65
2:B:306:PRO:HA	9:I:52:ARG:CG	2.26	0.65
2:O:414:ALA:O	2:O:418:VAL:HG23	1.96	0.65
2:B:56:ARG:HH12	2:B:172:LEU:HG	1.61	0.65
5:E:117:LEU:HD21	5:E:170:ARG:HD2	1.78	0.65
5:E:163:SER:HA	5:E:174:GLY:HA3	1.79	0.65
1:N:69:LYS:CD	1:N:70:ARG:HH21	2.03	0.65
7:T:50:PRO:HB2	7:T:51:PRO:CD	2.26	0.65
1:N:32:GLN:OE1	2:O:373:GLU:HG2	1.97	0.65
3:C:342:GLN:HE21	3:C:343:PRO:HD2	1.62	0.65
2:B:26:ILE:HD13	2:B:391:THR:HA	1.79	0.65
5:R:73:LYS:HB3	5:R:196:GLY:O	1.97	0.65
5:R:96:LEU:HD12	5:R:135:LEU:O	1.97	0.65
5:R:128:LYS:O	5:R:130:PRO:HD3	1.97	0.64
2:O:357:VAL:HG12	2:O:361:LYS:HE3	1.78	0.64
5:E:186:GLN:HG3	5:E:188:VAL:HG23	1.78	0.64
3:P:155:PRO:O	3:P:156:TYR:HB2	1.97	0.64
1:A:60:GLU:OE2	1:A:90:THR:HG22	1.98	0.64
3:C:9:HIS:O	3:C:13:LYS:HB3	1.96	0.64
5:R:101:ARG:HA	5:R:105:GLU:OE1	1.97	0.64
2:B:327:ILE:HD11	9:I:58:ARG:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:71:LEU:HD12	2:O:144:LEU:HD23	1.80	0.64
2:O:18:CYS:HB3	2:O:19:PRO:HD2	1.78	0.64
2:O:407:SER:O	2:O:411:VAL:HG23	1.98	0.64
5:E:78:LEU:HB3	5:E:132:TRP:CZ2	2.33	0.63
2:B:96:LEU:HB3	9:I:70:LEU:HD22	1.80	0.63
2:B:248:ASN:HD21	2:B:250:HIS:HB2	1.63	0.63
1:N:206:LYS:H	1:N:206:LYS:CD	2.10	0.63
4:D:175:THR:HG23	8:H:78:LYS:HD2	1.79	0.63
5:E:135:LEU:HD23	5:E:182:VAL:HG22	1.80	0.63
2:O:225:ASN:O	2:O:226:ILE:C	2.35	0.63
9:V:47:LEU:HD13	9:V:53:MET:HG2	1.80	0.63
2:B:169:LYS:HG3	2:B:240:TRP:HB2	1.81	0.63
4:Q:102:ARG:HA	4:Q:108:ALA:O	1.99	0.63
7:T:72:LYS:HG2	8:U:56:GLU:OE2	1.99	0.63
1:N:60:GLU:OE2	1:N:90:THR:HG22	1.98	0.63
8:U:43:ARG:HD2	8:U:47:ARG:NH2	2.14	0.63
1:N:112:LEU:O	1:N:116:VAL:HG23	1.99	0.62
2:O:47:ILE:HD13	2:O:120:MET:CE	2.29	0.62
9:V:1:AME:C	9:V:3:SER:H	2.12	0.62
3:P:236:MET:O	3:P:239:PRO:HD2	1.99	0.62
10:W:57:HIS:HA	10:W:60:GLU:OE2	1.99	0.62
1:N:35:CYS:SG	1:N:203:ILE:HD11	2.38	0.62
2:O:56:ARG:HH12	2:O:172:LEU:HG	1.64	0.62
2:O:22:GLU:HG2	2:O:39:GLU:HB3	1.80	0.62
2:O:306:PRO:HA	9:V:50:ARG:HG3	1.81	0.62
2:B:264:VAL:HG23	2:B:316:TYR:C	2.19	0.62
5:E:86:ASN:OD1	5:E:99:ARG:HB2	2.00	0.62
5:R:171:ILE:HD13	5:R:176:ALA:HB3	1.81	0.62
5:E:115:SER:HB2	5:E:116:LYS:HD2	1.81	0.62
5:E:119:ASP:HB3	5:E:179:ASN:CG	2.20	0.62
4:Q:134:TYR:CG	4:Q:162:PRO:HG3	2.35	0.62
2:B:47:ILE:HD13	2:B:120:MET:CE	2.30	0.61
7:T:46:PHE:O	7:T:50:PRO:HG2	2.00	0.61
5:R:102:THR:O	5:R:106:ILE:HG13	2.01	0.61
2:B:51:ILE:HG12	2:B:204:MET:HG2	1.82	0.61
4:Q:76:GLU:CD	4:Q:76:GLU:H	2.02	0.61
1:A:170:THR:HG22	1:A:171:THR:N	2.15	0.61
1:N:196:VAL:CG1	1:N:383:LEU:HD12	2.29	0.61
8:U:21:ARG:O	8:U:25:GLU:HG3	2.01	0.61
1:N:49:ASN:ND2	1:N:51:LYS:H	1.97	0.61
2:O:341:MET:CE	2:O:417:PHE:HE2	2.14	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:112:VAL:HG21	5:R:170:ARG:NH2	2.16	0.61
1:A:32:GLN:OE1	2:B:373:GLU:HG2	2.01	0.61
1:N:186:ILE:HG23	1:N:190:PHE:CD1	2.35	0.61
2:O:225:ASN:O	2:O:227:ARG:HB3	2.01	0.61
1:A:106:MET:HE2	1:A:107:PRO:HA	1.83	0.61
5:E:144:CYS:O	5:E:146:PRO:HD3	2.01	0.61
9:I:33:UNK:HG3	9:I:34:UNK:N	1.99	0.61
9:V:68:LEU:HD21	9:V:69:ASN:ND2	2.15	0.61
10:W:49:GLY:N	10:W:54:HIS:ND1	2.48	0.61
2:B:397:VAL:O	2:B:401:LYS:HG2	2.01	0.61
4:D:195:GLU:OE1	4:D:201:ARG:NH2	2.30	0.61
1:N:336:PHE:CE2	3:P:4:ASN:HB3	2.36	0.61
1:A:37:VAL:HG23	1:A:113:LEU:HD11	1.83	0.60
5:E:163:SER:H	5:E:175:PRO:HD2	1.66	0.60
2:O:51:ILE:HG12	2:O:204:MET:HG2	1.83	0.60
2:O:248:ASN:ND2	2:O:250:HIS:H	1.99	0.60
5:R:86:ASN:OD1	5:R:99:ARG:HB2	2.01	0.60
2:B:76:THR:CG2	2:B:82:SER:H	2.01	0.60
5:E:73:LYS:HB3	5:E:196:GLY:O	2.01	0.60
5:R:112:VAL:HG11	5:R:170:ARG:NH1	2.16	0.60
2:O:397:VAL:O	2:O:401:LYS:HG2	2.01	0.60
5:E:94:LYS:HD3	5:E:138:VAL:HG21	1.84	0.60
6:F:99:ARG:HH11	6:F:99:ARG:HG3	1.66	0.60
1:N:37:VAL:HG23	1:N:113:LEU:HD11	1.83	0.60
2:O:169:LYS:O	2:O:170:THR:HG23	2.01	0.60
2:B:385:GLU:HG2	9:I:2:LEU:HD13	1.81	0.60
1:N:395:TRP:HA	1:N:395:TRP:CE3	2.35	0.60
3:P:377:MET:HE2	6:S:20:TYR:HB2	1.84	0.60
4:D:47:ALA:N	4:D:50:ASN:HD22	1.87	0.60
1:A:102:LEU:HD13	1:A:105:ASP:OD2	2.02	0.60
2:B:43:PRO:O	2:B:113:ARG:HG3	2.00	0.60
2:B:341:MET:CE	2:B:417:PHE:HE2	2.15	0.60
5:E:190:ASP:C	5:E:192:LEU:H	2.04	0.60
2:B:33:LEU:HD21	2:B:224:LEU:HD12	1.82	0.60
2:O:248:ASN:HD21	2:O:428:GLY:HA2	1.67	0.60
4:Q:221:TYR:HD2	5:R:39:VAL:HG11	1.67	0.60
7:T:79:ASN:HD22	7:T:79:ASN:N	1.99	0.60
8:U:40:CYS:O	8:U:44:VAL:HG23	2.02	0.59
9:V:6:ALA:O	9:V:7:ARG:HG3	2.01	0.59
5:E:106:ILE:O	5:E:110:ALA:HB3	2.02	0.59
4:D:229:VAL:HG23	7:G:20:PRO:HG3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:168:TYR:CE2	2:O:172:LEU:HD12	2.37	0.59
2:O:29:LEU:HD11	2:O:221:GLU:HB3	1.83	0.59
2:O:341:MET:HE2	2:O:341:MET:CA	2.27	0.59
5:E:106:ILE:C	5:E:107:ASN:HD22	2.06	0.59
8:H:27:THR:HG22	8:H:29:LYS:N	2.16	0.59
9:I:70:LEU:HD23	9:I:71:ASN:N	2.17	0.59
2:O:374:THR:HG22	2:O:376:GLN:H	1.68	0.59
1:N:9:GLN:HG2	1:N:393:GLU:OE2	2.02	0.59
2:O:357:VAL:O	2:O:361:LYS:HG3	2.02	0.59
2:B:407:SER:O	2:B:411:VAL:HG23	2.01	0.59
8:H:21:ARG:O	8:H:25:GLU:HG3	2.02	0.59
2:B:314:VAL:HG13	9:I:63:ASP:HB3	1.83	0.59
4:Q:26:VAL:HG22	4:Q:188:THR:HG22	1.85	0.59
3:P:106:GLY:HA2	3:P:108:TYR:CE2	2.38	0.59
1:A:117:VAL:HG23	1:A:118:GLN:HG3	1.85	0.59
3:C:46:ILE:HA	12:C:501:HEM:HMC3	1.85	0.59
1:N:60:GLU:OE2	1:N:89:TYR:HA	2.03	0.59
2:O:101:THR:CG2	2:O:104:LYS:HE3	2.29	0.59
2:O:53:ALA:O	2:O:105:MET:HG3	2.03	0.59
5:R:186:GLN:HE21	5:R:188:VAL:HG13	1.67	0.59
1:A:222:THR:OG1	1:A:225:GLU:HG3	2.03	0.58
2:B:357:VAL:O	2:B:361:LYS:HG3	2.02	0.58
2:B:46:ARG:NH2	2:B:376:GLN:HG3	2.18	0.58
2:O:286:LYS:HE2	2:O:287:ARG:NH1	2.18	0.58
5:R:118:ARG:HB2	5:R:118:ARG:NH1	2.18	0.58
2:B:22:GLU:CG	2:B:23:ASP:H	1.99	0.58
2:B:248:ASN:HD21	2:B:428:GLY:HA2	1.68	0.58
4:Q:68:VAL:HG11	4:Q:92:PRO:HG3	1.84	0.58
6:S:77:LYS:HA	6:S:80:TRP:CE2	2.39	0.58
9:V:69:ASN:O	9:V:70:ALA:HB2	2.03	0.58
3:C:288:LYS:O	3:C:292:VAL:HG23	2.03	0.58
7:G:50:PRO:HB2	7:G:51:PRO:CD	2.32	0.58
1:N:382:HIS:ND1	1:N:389:ARG:HD2	2.17	0.58
4:Q:195:GLU:OE1	4:Q:201:ARG:NH2	2.35	0.58
2:B:248:ASN:ND2	2:B:428:GLY:HA2	2.19	0.58
4:Q:229:VAL:HG23	7:T:20:PRO:HG3	1.85	0.58
9:I:72:ALA:HB1	9:I:73:PRO:HD2	1.86	0.58
2:B:315:ASN:ND2	9:I:7:ARG:HD3	2.17	0.58
1:N:106:MET:HE2	1:N:107:PRO:HA	1.86	0.58
2:O:47:ILE:HD13	2:O:120:MET:HE2	1.86	0.58
3:P:69:HIS:CD2	3:P:73:ASN:HD22	2.22	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:160:LEU:HD12	9:I:64:LEU:HD13	1.85	0.58
3:P:145:THR:O	3:P:149:ASN:HB2	2.04	0.58
4:D:229:VAL:CG2	7:G:20:PRO:HG3	2.33	0.58
4:Q:150:ASN:O	4:Q:156:GLN:HA	2.04	0.58
4:D:54:VAL:HG12	4:D:55:THR:HG23	1.84	0.58
1:A:395:TRP:HA	1:A:395:TRP:CE3	2.39	0.57
2:B:207:VAL:HG21	2:B:383:GLY:CA	2.34	0.57
9:I:6:ALA:O	9:I:7:ARG:HG3	2.03	0.57
2:B:264:VAL:HG11	2:B:388:LEU:HD13	1.85	0.57
3:C:101:ARG:C	3:C:101:ARG:HD2	2.24	0.57
1:N:102:LEU:HD13	1:N:105:ASP:OD2	2.04	0.57
7:T:72:LYS:CE	8:U:57:GLU:OE1	2.51	0.57
2:B:374:THR:HG22	2:B:376:GLN:H	1.69	0.57
2:O:422:LYS:O	2:O:436:LEU:HD21	2.03	0.57
2:O:59:THR:HG22	2:O:60:THR:N	2.19	0.57
1:A:133:VAL:O	1:A:137:GLU:HG3	2.04	0.57
7:T:41:PHE:O	7:T:45:VAL:HG23	2.04	0.57
7:G:29:ILE:O	7:G:33:ALA:HB3	2.04	0.57
9:I:33:UNK:CG	9:I:34:UNK:H	2.03	0.57
1:N:117:VAL:HG23	1:N:118:GLN:HG3	1.86	0.57
1:N:402:VAL:HG22	1:N:406:MET:CE	2.35	0.57
5:R:49:TYR:CE1	10:W:32:GLU:HG3	2.40	0.57
3:P:5:ILE:O	3:P:5:ILE:HG22	2.05	0.57
2:B:381:GLU:OE1	9:I:3:SER:HB2	2.05	0.57
3:C:69:HIS:CD2	3:C:73:ASN:HD22	2.23	0.57
2:O:128:THR:HG21	2:O:224:LEU:HD22	1.87	0.57
4:D:22:ASP:HA	10:J:50:LYS:HB3	1.87	0.57
1:N:222:THR:OG1	1:N:225:GLU:HG3	2.04	0.57
5:R:113:ASP:HB2	5:R:116:LYS:HB2	1.85	0.57
1:A:362:ARG:O	1:A:365:MET:HG2	2.05	0.56
3:P:138:GLN:HB2	3:P:255:GLU:O	2.05	0.56
2:B:341:MET:HE2	2:B:341:MET:CA	2.28	0.56
2:B:368:TYR:HB2	9:I:1:AME:HE3	1.87	0.56
4:D:134:TYR:CG	4:D:162:PRO:HG3	2.41	0.56
1:N:21:ASN:HB3	1:N:219:VAL:HG22	1.86	0.56
1:N:4:TYR:HB2	2:O:114:ASP:OD1	2.05	0.56
2:O:35:ILE:HD13	2:O:217:LYS:HA	1.87	0.56
4:Q:229:VAL:CG2	7:T:20:PRO:HG3	2.35	0.56
10:W:60:GLU:O	10:W:61:ALA:HB2	2.06	0.56
1:A:137:GLU:O	1:A:141:MET:HG3	2.05	0.56
3:C:22:LEU:HD21	14:C:504:UQ:HM32	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:230:ILE:HG22	4:D:219:LEU:HD13	1.87	0.56
4:D:97:ASN:HB2	4:D:98:PRO:HD2	1.86	0.56
2:O:192:HIS:O	2:O:196:GLN:HG3	2.04	0.56
1:A:64:PHE:HE2	1:A:86:PHE:CZ	2.23	0.56
2:B:276:GLN:HG2	2:B:281:ALA:HB2	1.87	0.56
3:C:5:ILE:O	3:C:5:ILE:HG22	2.06	0.56
2:O:207:VAL:HG21	2:O:383:GLY:CA	2.35	0.56
5:R:117:LEU:HD21	5:R:172:ARG:HH11	1.70	0.56
2:B:53:ALA:O	2:B:105:MET:HG3	2.06	0.56
5:R:77:LYS:HE2	5:R:79:SER:HB2	1.88	0.56
2:O:182:ARG:HG2	2:O:182:ARG:HH11	1.70	0.56
4:Q:221:TYR:CD2	5:R:39:VAL:HG11	2.40	0.56
1:A:2:ALA:HB3	2:B:113:ARG:NH2	2.20	0.56
2:B:297:GLN:O	2:B:301:LYS:HG3	2.05	0.56
7:G:65:GLU:O	7:G:69:LEU:HG	2.06	0.56
1:N:90:THR:O	1:N:167:VAL:HG11	2.05	0.56
10:W:38:GLY:O	10:W:42:ILE:HG13	2.05	0.56
4:D:203:ARG:HB2	4:D:203:ARG:HH11	1.70	0.56
3:C:234:THR:HG21	4:D:219:LEU:HD12	1.88	0.56
2:O:273:SER:O	2:O:276:GLN:HB3	2.06	0.56
3:P:153:ALA:O	3:P:155:PRO:HD3	2.06	0.56
1:A:405:ARG:HG2	1:A:405:ARG:HH11	1.70	0.55
2:B:101:THR:CG2	2:B:104:LYS:HE3	2.33	0.55
2:B:31:ASN:N	2:B:31:ASN:ND2	2.52	0.55
4:Q:158:ILE:HG12	4:Q:160:MET:H	1.71	0.55
6:S:13:MET:O	6:S:16:ILE:HB	2.05	0.55
1:A:67:THR:HG21	1:A:115:ASP:CG	2.26	0.55
2:B:286:LYS:HE2	2:B:287:ARG:NH1	2.21	0.55
5:E:129:LYS:HG3	5:E:187:PHE:CE2	2.41	0.55
2:O:248:ASN:ND2	2:O:428:GLY:HA2	2.21	0.55
2:O:297:GLN:O	2:O:301:LYS:HG3	2.06	0.55
7:G:46:PHE:O	7:G:50:PRO:HG2	2.06	0.55
3:P:245:LEU:O	4:Q:201:ARG:HD2	2.05	0.55
5:R:134:ILE:HD11	5:R:193:VAL:HG21	1.88	0.55
3:P:230:ILE:HG23	16:R:502:PEE:H25	1.89	0.55
7:G:41:PHE:O	7:G:45:VAL:HG23	2.07	0.55
2:B:168:TYR:CE2	2:B:172:LEU:HD12	2.42	0.55
2:B:414:ALA:O	2:B:418:VAL:HG23	2.07	0.55
4:D:8:PRO:HG2	4:D:10:PHE:CE1	2.41	0.55
3:P:365:ILE:HG22	3:P:366:LEU:N	2.22	0.55
1:N:10:ASN:ND2	2:O:19:PRO:HB2	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:328:LEU:HD12	7:T:51:PRO:HB3	1.88	0.55
2:B:71:LEU:HD23	9:I:68:ILE:HG13	1.89	0.55
6:F:40:ASP:O	6:F:44:LYS:HG2	2.07	0.55
1:A:112:LEU:O	1:A:116:VAL:HG23	2.07	0.55
2:O:292:THR:HG22	2:O:292:THR:O	2.07	0.55
1:A:387:GLY:O	1:A:388:ARG:HB3	2.07	0.54
2:B:38:LEU:HG	2:B:39:GLU:N	2.21	0.54
1:N:40:TRP:CD1	1:N:96:ALA:HB2	2.42	0.54
8:U:43:ARG:HD2	8:U:47:ARG:HH22	1.72	0.54
5:E:129:LYS:HB3	5:E:132:TRP:HB2	1.88	0.54
5:E:189:GLY:O	5:E:192:LEU:N	2.39	0.54
1:N:134:ILE:HG22	1:N:174:ILE:HD13	1.89	0.54
1:N:344:ARG:HG3	1:N:344:ARG:HH11	1.72	0.54
7:T:72:LYS:HE2	8:U:57:GLU:OE1	2.07	0.54
9:V:47:LEU:HD11	9:V:56:ARG:HH11	1.72	0.54
6:F:77:LYS:HA	6:F:80:TRP:CE2	2.42	0.54
2:O:248:ASN:C	2:O:248:ASN:ND2	2.60	0.54
5:R:3:ASN:ND2	5:R:3:ASN:H	2.06	0.54
7:T:50:PRO:HB2	7:T:51:PRO:HD3	1.89	0.54
1:A:398:ARG:NH1	1:A:398:ARG:HG2	2.23	0.54
2:B:417:PHE:O	2:B:422:LYS:HE3	2.08	0.54
9:I:72:ALA:HB1	9:I:73:PRO:CD	2.38	0.54
1:N:294:LEU:HD11	1:N:334:MET:HE3	1.89	0.54
1:N:362:ARG:O	1:N:365:MET:HG2	2.08	0.54
5:R:3:ASN:HD22	5:R:3:ASN:H	1.55	0.54
1:N:67:THR:HG21	1:N:115:ASP:CG	2.27	0.54
4:Q:203:ARG:HB2	4:Q:203:ARG:HH11	1.73	0.54
2:B:166:ALA:O	2:B:242:GLY:N	2.35	0.54
3:C:145:THR:O	3:C:149:ASN:HB2	2.08	0.54
4:D:150:ASN:O	4:D:156:GLN:HA	2.06	0.54
5:E:129:LYS:CB	5:E:132:TRP:HB2	2.38	0.54
8:U:32:LYS:O	8:U:36:ARG:HG3	2.06	0.54
8:U:40:CYS:HA	8:U:43:ARG:NH1	2.23	0.54
1:A:336:PHE:CE2	3:C:4:ASN:HB3	2.43	0.54
7:G:50:PRO:HB2	7:G:51:PRO:HD3	1.90	0.54
3:P:344:VAL:HG12	3:P:349:ILE:HD11	1.90	0.54
5:R:126:ARG:NH2	5:R:169:GLY:O	2.41	0.54
6:S:40:ASP:O	6:S:44:LYS:HG2	2.06	0.54
5:E:169:GLY:O	5:E:179:ASN:HB3	2.07	0.54
5:E:194:VAL:O	5:E:194:VAL:HG12	2.07	0.54
2:O:160:LEU:HD12	9:V:62:LEU:HD13	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:168:TYR:HB2	2:O:173:ALA:HB2	1.89	0.54
2:O:227:ARG:HG3	2:O:228:SER:N	2.22	0.54
3:P:212:ILE:HD12	6:S:62:ILE:HG23	1.89	0.54
1:A:402:VAL:HG22	1:A:406:MET:CE	2.38	0.54
1:N:37:VAL:HG12	1:N:199:ALA:CB	2.38	0.54
1:N:395:TRP:HA	1:N:395:TRP:HE3	1.71	0.54
5:R:102:THR:OG1	5:R:105:GLU:HG3	2.07	0.54
5:R:83:GLU:HG3	5:R:100:HIS:CE1	2.43	0.54
2:O:307:PHE:H	9:V:50:ARG:HG2	1.72	0.54
2:B:168:TYR:HB2	2:B:173:ALA:HB2	1.89	0.54
7:T:65:GLU:O	7:T:69:LEU:HG	2.08	0.54
2:B:292:THR:O	2:B:292:THR:HG22	2.07	0.53
3:C:28:ILE:CD1	14:C:504:UQ:HM21	2.38	0.53
5:R:10:PHE:O	5:R:14:ARG:HG3	2.08	0.53
5:R:83:GLU:HB3	5:R:102:THR:CG2	2.27	0.53
5:E:3:ASN:HD22	5:E:3:ASN:H	1.56	0.53
1:N:64:PHE:HE2	1:N:86:PHE:CZ	2.26	0.53
4:Q:83:ARG:HH12	4:Q:86:LYS:HG3	1.73	0.53
2:B:147:ASP:OD1	9:I:68:ILE:HD11	2.08	0.53
3:C:245:LEU:O	4:D:201:ARG:HD2	2.08	0.53
5:E:109:GLU:OE2	5:E:166:ASP:HB2	2.08	0.53
2:O:27:THR:CG2	2:O:28:LYS:H	2.16	0.53
5:R:99:ARG:HB3	5:R:133:VAL:CG1	2.38	0.53
5:E:191:ASP:N	5:E:191:ASP:OD2	2.42	0.53
4:Q:97:ASN:HB2	4:Q:98:PRO:HD2	1.91	0.53
5:E:144:CYS:HB2	5:E:158:CYS:SG	2.48	0.53
7:G:79:ASN:N	7:G:79:ASN:ND2	2.56	0.53
5:R:76:ILE:HD12	5:R:98:VAL:HG21	1.90	0.53
6:S:99:ARG:HB3	6:S:99:ARG:NH1	2.23	0.53
2:B:124:LEU:HD11	2:B:223:PHE:CD2	2.43	0.53
5:E:95:PRO:HG2	5:E:145:VAL:HG11	1.89	0.53
2:O:402:ILE:HD13	2:O:402:ILE:C	2.28	0.53
2:O:417:PHE:O	2:O:422:LYS:HE3	2.09	0.53
3:P:243:LEU:HD12	3:P:243:LEU:O	2.08	0.53
5:R:78:LEU:HB3	5:R:132:TRP:HZ2	1.69	0.53
4:D:68:VAL:HG11	4:D:92:PRO:HG3	1.90	0.53
5:E:99:ARG:HB3	5:E:133:VAL:CG1	2.38	0.53
10:J:38:GLY:O	10:J:42:ILE:HG13	2.09	0.53
2:O:277:HIS:NE2	2:O:364:LEU:HD13	2.24	0.53
2:O:402:ILE:HD13	2:O:402:ILE:O	2.09	0.53
5:R:148:ALA:O	5:R:155:GLY:O	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:45:VAL:HG13	10:W:28:ALA:HA	1.91	0.53
7:T:79:ASN:N	7:T:79:ASN:ND2	2.54	0.53
2:B:166:ALA:HB2	2:B:244:ILE:HG13	1.90	0.53
2:B:199:PHE:O	2:B:226:ILE:HG21	2.08	0.53
2:B:35:ILE:O	2:B:213:HIS:HE1	1.92	0.53
5:R:166:ASP:OD1	5:R:168:SER:HB3	2.09	0.53
3:C:122:LEU:HD21	3:C:299:VAL:HG11	1.90	0.53
2:O:109:VAL:HG21	2:O:119:VAL:HG12	1.91	0.53
2:O:206:LEU:HD23	2:O:220:ALA:HB2	1.90	0.53
1:A:398:ARG:HH11	1:A:398:ARG:HG2	1.74	0.52
5:E:76:ILE:HD12	5:E:98:VAL:HG21	1.90	0.52
2:O:46:ARG:HH22	2:O:376:GLN:HG3	1.73	0.52
1:A:402:VAL:HG22	1:A:406:MET:HE2	1.91	0.52
2:B:277:HIS:NE2	2:B:364:LEU:HD13	2.24	0.52
3:C:2:ALA:HB3	3:C:8:SER:HB3	1.91	0.52
5:E:166:ASP:OD1	5:E:168:SER:HB3	2.08	0.52
5:E:96:LEU:HD21	5:E:195:VAL:HG21	1.91	0.52
2:O:219:VAL:O	2:O:223:PHE:HB2	2.09	0.52
2:O:57:TYR:CE2	2:O:203:ARG:NH2	2.73	0.52
3:P:230:ILE:HG22	4:Q:219:LEU:HD13	1.90	0.52
1:A:178:THR:CG2	1:A:179:ARG:N	2.73	0.52
2:B:29:LEU:HB3	2:B:30:PRO:HD2	1.91	0.52
3:C:106:GLY:HA2	3:C:108:TYR:CE2	2.43	0.52
5:E:134:ILE:HD11	5:E:193:VAL:HG21	1.91	0.52
7:G:79:ASN:N	7:G:79:ASN:HD22	2.07	0.52
5:R:155:GLY:HA3	5:R:166:ASP:C	2.30	0.52
2:B:132:PHE:CE1	2:B:191:LEU:HB3	2.45	0.52
2:B:71:LEU:HD12	2:B:144:LEU:HD23	1.92	0.52
2:B:207:VAL:HG12	2:B:208:GLY:N	2.25	0.52
9:I:49:LEU:HB3	9:I:55:MET:HG3	1.92	0.52
2:O:76:THR:CG2	2:O:82:SER:H	1.98	0.52
5:E:112:VAL:HG21	5:E:170:ARG:NH2	2.25	0.52
8:H:28:GLU:CG	8:H:32:LYS:HE3	2.39	0.52
2:O:424:MET:HB2	2:O:436:LEU:HD13	1.91	0.52
2:O:147:ASP:OD1	9:V:66:ILE:HD11	2.09	0.52
1:A:9:GLN:HG2	1:A:393:GLU:OE2	2.10	0.52
1:A:49:ASN:ND2	1:A:51:LYS:H	2.06	0.52
10:J:49:GLY:N	10:J:54:HIS:ND1	2.57	0.52
10:J:60:GLU:O	10:J:61:ALA:HB3	2.09	0.52
5:E:164:HIS:HD2	5:E:173:LYS:HB3	1.75	0.52
5:R:78:LEU:HD13	5:R:132:TRP:NE1	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:95:LYS:O	6:S:99:ARG:HG3	2.10	0.52
9:V:1:AME:C	9:V:3:SER:N	2.73	0.52
2:B:38:LEU:CG	2:B:39:GLU:N	2.72	0.52
2:B:402:ILE:HD13	2:B:402:ILE:C	2.30	0.52
3:P:342:GLN:NE2	3:P:343:PRO:HD2	2.23	0.52
2:B:132:PHE:CD1	2:B:191:LEU:HB3	2.45	0.52
4:D:238:ARG:CZ	5:E:5:VAL:HG22	2.40	0.52
1:N:49:ASN:HD21	1:N:51:LYS:H	1.58	0.52
2:O:314:VAL:CG1	9:V:61:ASP:HB3	2.38	0.52
1:A:40:TRP:CD1	1:A:96:ALA:HB2	2.45	0.51
7:G:48:VAL:O	7:G:51:PRO:HD2	2.10	0.51
1:N:134:ILE:CG2	1:N:174:ILE:HD13	2.40	0.51
1:N:178:THR:CG2	1:N:179:ARG:N	2.72	0.51
1:N:294:LEU:HD11	1:N:334:MET:CE	2.40	0.51
2:O:29:LEU:CD1	2:O:221:GLU:HB3	2.39	0.51
1:A:191:LYS:O	1:A:195:MET:HG3	2.10	0.51
3:C:202:HIS:NE2	14:C:504:UQ:O4	2.43	0.51
5:E:95:PRO:HG2	5:E:145:VAL:CG1	2.40	0.51
2:O:38:LEU:CG	2:O:39:GLU:N	2.73	0.51
3:P:347:PRO:O	3:P:350:ILE:HG22	2.10	0.51
3:P:380:TYR:OH	6:S:34:ASP:OD1	2.27	0.51
1:A:105:ASP:O	1:A:109:VAL:HG23	2.10	0.51
2:B:59:THR:HG22	2:B:60:THR:N	2.25	0.51
7:G:49:ALA:HB3	7:G:50:PRO:HD3	1.92	0.51
10:J:60:GLU:HA	10:J:60:GLU:OE2	2.09	0.51
6:S:13:MET:HA	6:S:16:ILE:CD1	2.37	0.51
5:E:107:ASN:N	5:E:107:ASN:ND2	2.51	0.51
8:U:27:THR:HG22	8:U:29:LYS:N	2.20	0.51
3:C:365:ILE:HG22	3:C:366:LEU:N	2.26	0.51
5:E:165:TYR:CD2	5:E:180:LEU:HG	2.45	0.51
1:N:321:GLY:HA2	1:N:342:TRP:HZ2	1.76	0.51
3:P:95:ILE:O	3:P:99:ILE:HG13	2.10	0.51
8:U:28:GLU:CG	8:U:32:LYS:HE3	2.40	0.51
3:C:6:ARG:HG2	3:C:16:ASN:HB2	1.93	0.51
1:N:133:VAL:O	1:N:137:GLU:HG3	2.10	0.51
1:N:137:GLU:O	1:N:141:MET:HG3	2.11	0.51
4:Q:57:THR:CG2	4:Q:58:GLU:N	2.74	0.51
7:T:3:HIS:O	7:T:7:LEU:HG	2.11	0.51
4:Q:44:ASP:OD1	4:Q:93:LYS:HE3	2.11	0.51
2:O:273:SER:OG	9:V:7:ARG:NH1	2.44	0.51
7:G:53:LEU:O	7:G:57:LEU:HG	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:402:VAL:HG22	1:N:406:MET:HE2	1.91	0.51
1:N:63:ALA:O	1:N:116:VAL:HG13	2.11	0.51
4:Q:237:TYR:HB2	6:S:60:PHE:CG	2.46	0.51
1:A:343:MET:HB3	1:A:444:ILE:HA	1.92	0.51
5:E:165:TYR:HA	5:E:170:ARG:O	2.11	0.51
5:R:96:LEU:HD21	5:R:195:VAL:HG21	1.92	0.51
7:T:34:LEU:HB2	7:T:35:PRO:HD3	1.93	0.51
2:B:273:SER:OG	9:I:7:ARG:NH1	2.44	0.51
8:H:12:GLU:HG2	8:H:13:LEU:N	2.25	0.51
2:B:287:ARG:HD3	9:I:53:GLU:HG2	1.92	0.50
1:N:75:PHE:O	1:N:79:VAL:HG23	2.11	0.50
2:O:357:VAL:CG1	2:O:361:LYS:HE3	2.41	0.50
1:A:395:TRP:HA	1:A:395:TRP:HE3	1.74	0.50
2:B:150:VAL:HG23	2:B:151:ALA:N	2.26	0.50
2:O:276:GLN:HG2	2:O:281:ALA:HB2	1.92	0.50
7:T:80:ASP:C	8:U:47:ARG:HD3	2.30	0.50
1:A:85:HIS:HB2	1:A:100:LYS:HB2	1.92	0.50
2:B:57:TYR:CE2	2:B:203:ARG:NH2	2.76	0.50
2:B:50:PHE:CD1	2:B:50:PHE:N	2.79	0.50
5:E:147:ILE:HG22	5:E:149:ASN:H	1.76	0.50
5:E:3:ASN:H	5:E:3:ASN:ND2	2.09	0.50
7:G:24:ARG:HB2	7:G:27:PRO:HB3	1.93	0.50
4:Q:57:THR:HG22	4:Q:58:GLU:N	2.27	0.50
10:W:58:LYS:HB2	10:W:59:TYR:CE1	2.45	0.50
2:O:47:ILE:HD11	2:O:116:VAL:CG1	2.42	0.50
2:O:38:LEU:HG	2:O:39:GLU:N	2.21	0.50
3:P:198:LEU:HD21	12:P:502:HEM:HMA3	1.94	0.50
4:Q:68:VAL:HG11	4:Q:92:PRO:CG	2.41	0.50
5:E:122:HIS:HE1	5:E:124:LEU:HD12	1.77	0.50
9:I:49:LEU:HD11	9:I:58:ARG:HH11	1.74	0.50
3:P:50:LEU:O	3:P:54:MET:HG3	2.11	0.50
1:A:35:CYS:SG	1:A:203:ILE:HD11	2.52	0.50
1:A:405:ARG:HD3	1:A:409:ASP:OD2	2.11	0.50
4:D:74:PRO:HB2	4:D:78:GLY:HA2	1.93	0.50
5:E:52:LYS:C	5:E:52:LYS:HD3	2.31	0.50
1:N:343:MET:HB3	1:N:444:ILE:HA	1.93	0.50
2:O:307:PHE:CD1	2:O:308:ASP:N	2.80	0.50
3:P:328:LEU:CD1	7:T:51:PRO:HB3	2.41	0.50
4:Q:74:PRO:HB2	4:Q:78:GLY:HA2	1.94	0.50
5:R:112:VAL:HG11	5:R:170:ARG:CZ	2.42	0.50
4:D:75:ASP:OD2	4:D:79:GLU:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:405:ARG:HG2	1:N:405:ARG:HH11	1.77	0.50
1:N:85:HIS:HB2	1:N:100:LYS:HB2	1.93	0.50
10:W:14:PHE:CD2	10:W:14:PHE:N	2.79	0.50
3:C:147:ILE:HG13	13:C:503:WF3:H15	1.94	0.50
2:B:206:LEU:HG	2:B:206:LEU:O	2.12	0.50
2:B:341:MET:HE1	2:B:417:PHE:HE2	1.76	0.50
9:I:49:LEU:HB3	9:I:55:MET:CG	2.42	0.50
10:W:22:LEU:O	10:W:22:LEU:HD23	2.12	0.50
1:A:40:TRP:CZ3	1:A:198:ALA:HB3	2.47	0.49
9:I:65:VAL:HG12	9:I:66:ALA:N	2.26	0.49
6:S:91:GLU:O	6:S:95:LYS:HG3	2.11	0.49
1:A:60:GLU:OE2	1:A:89:TYR:HA	2.12	0.49
7:G:81:GLN:HG3	7:G:81:GLN:OXT	2.11	0.49
3:P:321:LEU:HB2	3:P:374:GLU:OE1	2.12	0.49
4:Q:16:GLY:CA	4:Q:19:SER:OG	2.60	0.49
2:O:315:ASN:HD21	9:V:7:ARG:HH11	1.60	0.49
5:E:83:GLU:HB3	5:E:102:THR:CG2	2.31	0.49
6:F:73:ARG:NH1	7:G:32:ASP:OD2	2.44	0.49
2:B:368:TYR:HB2	9:I:1:AME:CE	2.42	0.49
2:O:287:ARG:HD3	9:V:51:GLU:HG2	1.93	0.49
2:O:399:ALA:HA	2:O:402:ILE:HG22	1.94	0.49
5:R:118:ARG:CB	5:R:118:ARG:HH11	2.26	0.49
5:R:165:TYR:HA	5:R:170:ARG:O	2.12	0.49
7:T:48:VAL:O	7:T:51:PRO:HD2	2.11	0.49
1:A:95:THR:HG22	1:A:96:ALA:N	2.27	0.49
2:B:27:THR:CG2	2:B:28:LYS:H	2.21	0.49
2:O:71:LEU:HD23	9:V:66:ILE:HG13	1.94	0.49
2:O:73:SER:N	2:O:74:PRO:HD2	2.28	0.49
3:P:208:ASN:HB2	3:P:209:PRO:HD2	1.94	0.49
4:Q:168:ILE:HG12	4:Q:168:ILE:O	2.12	0.49
2:B:307:PHE:CD1	2:B:308:ASP:N	2.81	0.49
12:C:502:HEM:HMC2	12:C:502:HEM:HBC2	1.93	0.49
3:P:288:LYS:O	3:P:292:VAL:HG23	2.12	0.49
5:R:164:HIS:HD2	5:R:173:LYS:HB3	1.76	0.49
2:B:262:ALA:CB	2:B:269:ALA:HA	2.43	0.49
3:C:173:ASN:N	3:C:174:PRO:HD2	2.27	0.49
3:C:342:GLN:NE2	3:C:343:PRO:HD2	2.26	0.49
5:E:107:ASN:O	5:E:111:GLU:HG3	2.13	0.49
8:H:18:THR:O	8:H:22:GLU:HG3	2.13	0.49
2:O:268:GLU:HG2	2:O:272:PHE:CE1	2.47	0.49
5:R:109:GLU:CG	5:R:123:ASP:HB2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:133:VAL:HG13	5:R:133:VAL:O	2.12	0.49
1:N:61:HIS:CE1	1:N:134:ILE:HG12	2.47	0.49
1:A:134:ILE:CG2	1:A:174:ILE:HD13	2.42	0.49
1:A:196:VAL:CG1	1:A:383:LEU:HD12	2.42	0.49
1:A:293:ARG:HD3	1:A:344:ARG:NH1	2.27	0.49
2:B:315:ASN:HD21	9:I:7:ARG:HH11	1.61	0.49
2:B:344:LEU:HD13	2:B:417:PHE:CE2	2.47	0.49
2:O:341:MET:HE3	2:O:417:PHE:CE2	2.48	0.49
2:B:398:VAL:HG13	2:B:399:ALA:N	2.28	0.49
4:D:166:ASN:ND2	4:D:166:ASN:H	2.10	0.49
5:E:141:HIS:HB2	5:E:176:ALA:HB2	1.94	0.49
1:N:219:VAL:HG12	1:N:220:SER:N	2.27	0.49
2:B:248:ASN:ND2	2:B:250:HIS:H	2.11	0.49
2:O:306:PRO:HA	9:V:50:ARG:CG	2.43	0.49
2:O:345:LYS:O	2:O:349:GLN:HG3	2.13	0.49
3:P:334:LEU:HD21	16:P:507:PEE:H65	1.95	0.49
5:R:114:VAL:HG12	5:R:114:VAL:O	2.13	0.49
2:B:273:SER:O	2:B:276:GLN:HB3	2.13	0.48
2:B:314:VAL:CG1	9:I:63:ASP:HB3	2.42	0.48
1:N:41:ILE:HD13	1:N:190:PHE:CD2	2.48	0.48
1:N:35:CYS:HB2	1:N:200:ALA:O	2.13	0.48
3:P:33:ASN:HB3	21:P:608:HOH:O	2.13	0.48
3:P:234:THR:HG21	4:Q:219:LEU:HD12	1.95	0.48
4:Q:26:VAL:HG12	4:Q:55:THR:HG21	1.95	0.48
5:R:186:GLN:HE21	5:R:188:VAL:CG1	2.25	0.48
5:E:129:LYS:HD2	5:E:132:TRP:HD1	1.78	0.48
5:E:137:GLY:O	5:E:145:VAL:HG13	2.13	0.48
5:E:155:GLY:HA3	5:E:166:ASP:C	2.34	0.48
5:E:75:GLU:HB3	5:E:194:VAL:HG22	1.95	0.48
1:A:134:ILE:HG22	1:A:174:ILE:HD13	1.94	0.48
1:A:37:VAL:HG12	1:A:199:ALA:CB	2.42	0.48
5:R:118:ARG:CB	5:R:118:ARG:NH1	2.77	0.48
6:S:73:ARG:NH1	7:T:32:ASP:OD2	2.46	0.48
8:U:28:GLU:O	8:U:32:LYS:HG3	2.14	0.48
2:B:109:VAL:HG21	2:B:119:VAL:HG12	1.94	0.48
2:B:27:THR:CG2	2:B:28:LYS:N	2.76	0.48
2:B:372:VAL:HG13	2:B:378:LEU:HA	1.95	0.48
5:E:84:GLY:CA	5:E:102:THR:HG23	2.42	0.48
7:G:3:HIS:O	7:G:7:LEU:HG	2.14	0.48
2:O:344:LEU:HD13	2:O:417:PHE:CE2	2.48	0.48
5:R:29:SER:HA	5:R:32:ARG:NH2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:67:ASP:CG	6:S:71:LYS:HZ3	2.16	0.48
9:V:33:UNK:C	9:V:71:PRO:HG2	2.43	0.48
2:B:402:ILE:HD13	2:B:402:ILE:O	2.14	0.48
5:E:130:PRO:HG2	5:E:131:GLU:H	1.79	0.48
5:E:78:LEU:HD11	5:E:187:PHE:CE2	2.48	0.48
2:B:424:MET:HB2	2:B:436:LEU:HD13	1.95	0.48
1:N:111:GLU:HG3	1:N:215:HIS:CD2	2.49	0.48
1:N:122:LEU:HD11	1:N:186:ILE:HD12	1.96	0.48
4:Q:151:PRO:HA	4:Q:156:GLN:HG3	1.94	0.48
5:R:107:ASN:O	5:R:110:ALA:N	2.43	0.48
9:V:47:LEU:HB3	9:V:53:MET:CG	2.44	0.48
2:B:56:ARG:HG3	2:B:171:ALA:HB1	1.96	0.48
2:B:370:MET:O	2:B:373:GLU:HG3	2.14	0.48
2:B:38:LEU:O	2:B:39:GLU:HB2	2.14	0.48
1:A:321:GLY:HA2	1:A:342:TRP:HZ2	1.79	0.48
2:B:192:HIS:O	2:B:196:GLN:HG3	2.14	0.48
2:B:248:ASN:ND2	2:B:248:ASN:C	2.67	0.48
2:B:274:VAL:O	2:B:278:VAL:HG23	2.14	0.48
2:B:357:VAL:CG1	2:B:361:LYS:HE3	2.41	0.48
5:E:86:ASN:HB2	5:E:99:ARG:HE	1.79	0.48
5:E:76:ILE:CD1	5:E:98:VAL:HG21	2.43	0.48
8:U:73:LEU:HD12	8:U:73:LEU:O	2.13	0.48
1:A:170:THR:HG22	1:A:172:GLU:H	1.79	0.48
2:B:47:ILE:HD11	2:B:116:VAL:CG1	2.43	0.48
3:C:321:LEU:HB2	3:C:374:GLU:OE1	2.14	0.48
5:E:81:ILE:HG22	5:E:100:HIS:HB2	1.95	0.48
5:E:119:ASP:O	5:E:121:GLN:N	2.46	0.48
1:N:342:TRP:O	1:N:345:LEU:HB2	2.12	0.48
2:O:29:LEU:HB3	2:O:30:PRO:CD	2.43	0.48
5:R:194:VAL:HG12	5:R:194:VAL:O	2.14	0.48
2:O:76:THR:HG23	2:O:136:GLU:OE1	2.13	0.48
2:O:268:GLU:HG2	2:O:272:PHE:HE1	1.78	0.48
2:O:372:VAL:HG13	2:O:378:LEU:HA	1.95	0.48
8:U:36:ARG:HH11	8:U:36:ARG:CB	2.08	0.48
1:A:178:THR:HG22	1:A:179:ARG:N	2.29	0.47
1:A:382:HIS:ND1	1:A:389:ARG:HD2	2.29	0.47
9:I:1:AME:C	9:I:3:SER:H	2.27	0.47
2:O:38:LEU:O	2:O:39:GLU:HB2	2.14	0.47
4:Q:47:ALA:N	4:Q:50:ASN:HD22	1.85	0.47
4:Q:54:VAL:HG12	4:Q:55:THR:HG23	1.96	0.47
7:T:49:ALA:HB3	7:T:50:PRO:HD3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:80:ALA:HA	2:B:84:ARG:NH1	2.21	0.47
4:D:57:THR:CG2	4:D:58:GLU:N	2.76	0.47
8:H:35:GLU:O	8:H:39:LEU:HG	2.14	0.47
3:P:6:ARG:HG2	3:P:16:ASN:HB2	1.96	0.47
1:A:7:THR:HG21	2:B:113:ARG:HD2	1.96	0.47
2:B:225:ASN:O	2:B:226:ILE:C	2.52	0.47
2:B:307:PHE:N	9:I:52:ARG:HG2	2.27	0.47
1:N:433:ASP:OD2	1:N:435:ASN:HB2	2.14	0.47
2:O:403:ASP:C	2:O:405:VAL:H	2.16	0.47
2:O:341:MET:HE1	2:O:417:PHE:HE2	1.78	0.47
3:P:332:ASN:ND2	3:P:358:SER:OG	2.47	0.47
5:R:166:ASP:OD2	5:R:172:ARG:HD3	2.13	0.47
2:O:156:GLN:NE2	9:V:75:ARG:C	2.68	0.47
1:A:170:THR:CG2	1:A:171:THR:N	2.78	0.47
2:B:402:ILE:O	2:B:405:VAL:HG23	2.13	0.47
3:C:103:LEU:HD12	3:C:103:LEU:O	2.13	0.47
3:C:344:VAL:HG12	3:C:349:ILE:HD11	1.97	0.47
1:N:387:GLY:O	1:N:388:ARG:HB3	2.13	0.47
2:O:132:PHE:CE1	2:O:191:LEU:HB3	2.49	0.47
2:O:71:LEU:CD1	2:O:144:LEU:HD23	2.43	0.47
2:O:166:ALA:HB2	2:O:244:ILE:HG13	1.96	0.47
2:B:207:VAL:HG12	2:B:208:GLY:H	1.79	0.47
1:N:228:VAL:O	1:N:228:VAL:HG13	2.13	0.47
5:R:171:ILE:CD1	5:R:176:ALA:HB3	2.45	0.47
5:E:161:HIS:HB2	5:E:175:PRO:HG3	1.96	0.47
7:G:34:LEU:HB2	7:G:35:PRO:HD3	1.96	0.47
1:N:170:THR:CG2	1:N:171:THR:N	2.76	0.47
5:R:129:LYS:HG2	5:R:131:GLU:OE1	2.14	0.47
6:S:16:ILE:O	6:S:19:TRP:HB3	2.15	0.47
1:A:228:VAL:O	1:A:228:VAL:HG13	2.14	0.47
1:N:317:THR:HG23	1:N:318:GLY:N	2.30	0.47
2:O:207:VAL:HG12	2:O:208:GLY:N	2.30	0.47
3:P:34:PHE:HB2	21:P:601:HOH:O	2.14	0.47
6:S:13:MET:HE3	6:S:17:ARG:HH12	1.80	0.47
2:B:403:ASP:C	2:B:405:VAL:H	2.18	0.47
3:C:138:GLN:HB2	3:C:255:GLU:O	2.15	0.47
5:E:166:ASP:OD2	5:E:170:ARG:HB2	2.14	0.47
8:H:26:GLN:HA	8:H:26:GLN:OE1	2.14	0.47
1:N:18:THR:HG23	1:N:24:ARG:CG	2.40	0.47
1:N:37:VAL:HG12	1:N:199:ALA:HB1	1.97	0.47
1:N:321:GLY:HA2	1:N:342:TRP:CZ2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:166:ALA:O	2:O:242:GLY:N	2.45	0.47
6:S:13:MET:CE	6:S:17:ARG:HH12	2.27	0.47
6:S:70:LEU:HD12	6:S:70:LEU:C	2.35	0.47
5:E:116:LYS:HD2	5:E:116:LYS:N	2.13	0.47
5:E:127:VAL:HG12	5:E:128:LYS:N	2.30	0.47
1:A:75:PHE:O	1:A:79:VAL:HG23	2.15	0.47
3:C:156:TYR:N	3:C:156:TYR:CD2	2.81	0.47
3:C:243:LEU:HD12	3:C:243:LEU:O	2.14	0.47
2:O:150:VAL:HG23	2:O:151:ALA:N	2.29	0.47
2:O:235:ALA:O	2:O:236:LYS:C	2.53	0.47
5:R:100:HIS:HA	5:R:131:GLU:O	2.14	0.47
4:D:221:TYR:CD2	5:E:39:VAL:HG11	2.50	0.47
5:E:133:VAL:HG13	5:E:133:VAL:O	2.15	0.47
2:O:398:VAL:HG13	2:O:399:ALA:N	2.30	0.47
5:R:156:TYR:N	5:R:165:TYR:O	2.37	0.47
5:R:165:TYR:CD2	5:R:180:LEU:HG	2.50	0.47
4:Q:235:MET:HE1	6:S:64:ARG:N	2.30	0.47
5:R:49:TYR:HE1	10:W:32:GLU:HG3	1.78	0.47
5:E:151:GLY:HA2	5:E:157:TYR:HB2	1.96	0.46
1:N:156:THR:HA	5:R:7:VAL:HG21	1.96	0.46
1:N:23:LEU:HA	1:N:192:ALA:O	2.16	0.46
2:O:28:LYS:CE	2:O:32:GLY:HA2	2.45	0.46
9:V:47:LEU:HB3	9:V:53:MET:HG3	1.95	0.46
2:B:235:ALA:O	2:B:236:LYS:C	2.53	0.46
2:B:46:ARG:HH22	2:B:376:GLN:HG3	1.80	0.46
1:N:40:TRP:CZ3	1:N:198:ALA:HB3	2.50	0.46
2:O:73:SER:N	2:O:74:PRO:CD	2.78	0.46
3:P:147:ILE:HG13	13:P:504:WF3:H15	1.97	0.46
3:P:146:VAL:HG12	3:P:147:ILE:N	2.31	0.46
4:Q:75:ASP:OD2	4:Q:79:GLU:HB2	2.15	0.46
5:R:52:LYS:HD3	5:R:52:LYS:C	2.35	0.46
6:S:52:GLU:OE2	7:T:11:ARG:NH1	2.48	0.46
3:C:19:LEU:C	3:C:20:ILE:HG13	2.36	0.46
3:C:266:PRO:HA	3:C:267:PRO:HD3	1.79	0.46
4:D:158:ILE:HG12	4:D:160:MET:H	1.80	0.46
4:D:168:ILE:HG12	4:D:168:ILE:O	2.15	0.46
4:D:16:GLY:N	4:D:19:SER:OG	2.49	0.46
6:F:52:GLU:OE2	7:G:11:ARG:NH1	2.44	0.46
2:O:282:GLY:HA2	2:O:283:PRO:HD2	1.74	0.46
5:R:83:GLU:OE1	5:R:103:GLN:NE2	2.49	0.46
1:A:186:ILE:HG23	1:A:190:PHE:HD1	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:TRP:O	1:A:345:LEU:HB2	2.16	0.46
2:B:286:LYS:HE2	2:B:287:ARG:CZ	2.45	0.46
3:C:146:VAL:HG12	3:C:147:ILE:N	2.30	0.46
5:E:102:THR:HB	5:E:103:GLN:OE1	2.15	0.46
5:E:104:ALA:O	5:E:108:GLN:HB3	2.15	0.46
5:E:134:ILE:O	5:E:182:VAL:HG13	2.15	0.46
5:E:29:SER:HA	5:E:32:ARG:NH2	2.30	0.46
2:O:67:HIS:O	2:O:70:ARG:HB3	2.15	0.46
3:P:98:HIS:CD2	12:P:502:HEM:NC	2.83	0.46
4:Q:13:SER:O	10:W:50:LYS:NZ	2.46	0.46
9:V:2:LEU:HD12	9:V:2:LEU:H	1.78	0.46
2:B:230:ALA:O	2:B:231:GLY:C	2.54	0.46
4:D:57:THR:CG2	4:D:59:ALA:H	2.23	0.46
3:P:101:ARG:HD2	3:P:102:GLY:N	2.31	0.46
1:A:15:ASN:O	1:A:26:ALA:HA	2.16	0.46
1:A:294:LEU:HD11	1:A:334:MET:CE	2.46	0.46
1:A:294:LEU:HD11	1:A:334:MET:HE3	1.98	0.46
2:B:141:GLN:N	2:B:142:PRO:HD2	2.31	0.46
2:B:86:THR:O	2:B:90:GLU:HG3	2.15	0.46
5:E:186:GLN:O	5:E:193:VAL:HA	2.16	0.46
9:I:49:LEU:CD1	9:I:55:MET:HG2	2.44	0.46
1:N:178:THR:HG22	1:N:179:ARG:N	2.30	0.46
4:Q:22:ASP:HA	10:W:50:LYS:HB3	1.98	0.46
3:C:157:ILE:O	3:C:157:ILE:HG12	2.15	0.46
4:D:239:PRO:C	4:D:241:LYS:H	2.18	0.46
7:T:53:LEU:O	7:T:57:LEU:HG	2.15	0.46
1:A:405:ARG:HG2	1:A:405:ARG:NH1	2.30	0.46
3:C:334:LEU:HD21	16:C:506:PEE:H65	1.97	0.46
2:O:132:PHE:CD1	2:O:191:LEU:HB3	2.51	0.46
2:O:35:ILE:O	2:O:213:HIS:HE1	1.98	0.46
2:B:46:ARG:HD2	2:B:110:GLU:HG2	1.97	0.46
2:B:63:LEU:HB2	2:B:182:ARG:CD	2.42	0.46
5:E:90:LYS:HE3	5:E:93:GLY:HA2	1.96	0.46
6:F:16:ILE:O	6:F:19:TRP:HB3	2.16	0.46
1:N:369:LEU:HD12	1:N:392:LEU:HD11	1.98	0.46
4:Q:116:ILE:HG23	4:Q:117:VAL:N	2.31	0.46
2:B:76:THR:HG23	2:B:82:SER:HB2	1.98	0.46
3:C:328:LEU:CD1	7:G:51:PRO:HB3	2.46	0.46
7:T:36:ASN:OD1	7:T:39:ARG:NH1	2.49	0.46
1:A:307:PHE:C	1:A:307:PHE:CD1	2.89	0.45
4:D:208:MET:O	4:D:212:SER:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:398:ARG:HG2	1:N:398:ARG:NH1	2.30	0.45
2:O:201:SER:H	2:O:227:ARG:HA	1.81	0.45
2:O:201:SER:HB3	2:O:227:ARG:HB2	1.98	0.45
9:V:63:VAL:HG12	9:V:64:ALA:N	2.31	0.45
6:F:77:LYS:HE2	6:F:77:LYS:HB3	1.71	0.45
1:N:106:MET:HG3	1:N:203:ILE:HG21	1.98	0.45
5:R:109:GLU:HA	5:R:109:GLU:OE2	2.17	0.45
6:S:76:PRO:HD2	6:S:79:GLN:OE1	2.16	0.45
1:A:354:VAL:HG23	1:A:355:LYS:N	2.32	0.45
2:B:262:ALA:O	2:B:320:GLY:HA3	2.16	0.45
3:C:156:TYR:C	3:C:158:GLY:H	2.19	0.45
1:N:264:ASP:HA	1:N:265:PRO:HD3	1.76	0.45
1:N:307:PHE:CD1	1:N:307:PHE:C	2.88	0.45
8:U:27:THR:O	8:U:31:VAL:HG23	2.17	0.45
1:A:272:VAL:O	1:A:275:ALA:HB3	2.17	0.45
2:B:345:LYS:O	2:B:349:GLN:HG3	2.16	0.45
3:C:158:GLY:O	3:C:160:THR:N	2.49	0.45
4:D:235:MET:HE1	6:F:64:ARG:HA	1.99	0.45
4:D:65:ALA:O	4:D:85:GLY:HA3	2.16	0.45
5:E:185:TYR:O	5:E:186:GLN:HB3	2.16	0.45
10:J:4:ALA:O	10:J:8:GLN:HG3	2.17	0.45
2:O:33:LEU:CD2	2:O:224:LEU:HD12	2.46	0.45
8:U:21:ARG:HG3	8:U:21:ARG:HH11	1.80	0.45
3:C:109:LEU:HA	3:C:109:LEU:HD23	1.74	0.45
3:C:122:LEU:HD21	3:C:299:VAL:CG1	2.47	0.45
3:C:69:HIS:HD2	3:C:73:ASN:HD22	1.65	0.45
10:J:14:PHE:CD2	10:J:14:PHE:N	2.82	0.45
2:B:203:ARG:HD2	2:B:230:ALA:HA	1.98	0.45
2:B:25:GLU:HB2	2:B:213:HIS:CG	2.52	0.45
2:O:305:GLN:HB3	2:O:306:PRO:HD2	1.99	0.45
2:O:46:ARG:HD2	2:O:110:GLU:HG2	1.98	0.45
5:R:136:VAL:O	5:R:138:VAL:N	2.46	0.45
2:B:341:MET:HE3	2:B:417:PHE:HE2	1.82	0.45
4:Q:169:LEU:HD23	4:Q:169:LEU:C	2.38	0.45
1:A:130:GLU:O	1:A:134:ILE:HG13	2.17	0.45
2:B:368:TYR:O	2:B:372:VAL:HG23	2.17	0.45
3:C:31:TRP:CZ3	16:C:506:PEE:H20	2.52	0.45
1:A:136:GLN:NE2	9:I:50:LEU:HB3	2.32	0.45
1:N:231:LEU:CD2	1:N:232:PRO:HD2	2.47	0.45
1:N:395:TRP:CE3	1:N:398:ARG:HD2	2.52	0.45
2:O:166:ALA:HB1	2:O:242:GLY:C	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:286:LYS:HE2	2:O:287:ARG:CZ	2.47	0.45
2:O:286:LYS:O	2:O:287:ARG:HB2	2.17	0.45
3:P:328:LEU:HD12	3:P:328:LEU:HA	1.80	0.45
4:Q:214:LEU:O	4:Q:218:LEU:HG	2.17	0.45
1:A:122:LEU:HD11	1:A:186:ILE:HD12	1.99	0.45
3:C:342:GLN:HA	3:C:342:GLN:NE2	2.32	0.45
6:F:67:ASP:CG	6:F:71:LYS:HZ3	2.20	0.45
6:F:70:LEU:HD12	6:F:70:LEU:C	2.36	0.45
7:G:36:ASN:OD1	7:G:39:ARG:NH1	2.50	0.45
8:H:40:CYS:HA	8:H:43:ARG:NH1	2.32	0.45
5:R:130:PRO:C	5:R:132:TRP:H	2.20	0.45
1:A:90:THR:O	1:A:167:VAL:HG11	2.17	0.45
2:B:277:HIS:CD2	2:B:364:LEU:HB2	2.52	0.45
3:C:155:PRO:O	3:C:157:ILE:HG22	2.16	0.45
6:F:32:MET:HE3	6:F:87:LYS:HE3	1.99	0.45
7:G:71:ARG:NH1	8:H:56:GLU:HG3	2.32	0.45
5:E:45:VAL:HG13	10:J:28:ALA:HA	1.99	0.45
1:N:106:MET:HG3	1:N:203:ILE:CD1	2.38	0.45
3:P:122:LEU:HD21	3:P:299:VAL:HG11	1.98	0.45
4:Q:16:GLY:N	4:Q:19:SER:OG	2.50	0.45
10:W:57:HIS:CE1	10:W:58:LYS:HG3	2.52	0.45
2:B:46:ARG:HD2	2:B:110:GLU:CD	2.38	0.44
3:C:122:LEU:CD2	3:C:299:VAL:HG11	2.46	0.44
12:C:502:HEM:HMC2	12:C:502:HEM:CBC	2.47	0.44
5:E:100:HIS:HA	5:E:131:GLU:O	2.17	0.44
1:N:10:ASN:OD1	2:O:18:CYS:HB3	2.16	0.44
2:O:56:ARG:HG3	2:O:171:ALA:HB1	1.99	0.44
3:P:287:ASN:O	3:P:288:LYS:C	2.56	0.44
3:P:31:TRP:CZ3	16:P:507:PEE:H20	2.51	0.44
7:T:73:ASN:HD21	7:T:75:ALA:HB3	1.82	0.44
1:A:321:GLY:HA2	1:A:342:TRP:CZ2	2.52	0.44
4:D:169:LEU:HD23	4:D:169:LEU:C	2.38	0.44
1:N:405:ARG:HD3	1:N:409:ASP:OD2	2.18	0.44
2:O:277:HIS:CD2	2:O:364:LEU:HB2	2.52	0.44
9:V:47:LEU:CD1	9:V:53:MET:HG2	2.46	0.44
10:W:20:PHE:C	10:W:20:PHE:CD1	2.90	0.44
1:A:264:ASP:HA	1:A:265:PRO:HD3	1.75	0.44
1:A:269:VAL:HG21	1:A:410:VAL:HG21	2.00	0.44
2:B:200:THR:OG1	2:B:203:ARG:HD3	2.17	0.44
5:E:171:ILE:HG12	5:E:176:ALA:O	2.18	0.44
3:C:328:LEU:HD12	7:G:51:PRO:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:109:VAL:HA	1:N:112:LEU:HD12	1.99	0.44
2:O:305:GLN:HB3	2:O:306:PRO:CD	2.48	0.44
9:V:69:ASN:O	9:V:70:ALA:CB	2.65	0.44
1:A:82:MET:HE3	1:A:105:ASP:HB3	1.99	0.44
3:C:215:ASP:HB3	7:G:8:ALA:HB2	2.00	0.44
5:E:74:ILE:CG2	5:E:195:VAL:HB	2.47	0.44
1:N:15:ASN:O	1:N:26:ALA:HA	2.18	0.44
2:O:221:GLU:CG	2:O:222:GLN:H	2.25	0.44
2:O:248:ASN:HD22	2:O:250:HIS:H	1.63	0.44
2:O:50:PHE:CD1	2:O:50:PHE:N	2.85	0.44
5:R:122:HIS:O	5:R:124:LEU:N	2.51	0.44
2:O:150:VAL:CG2	2:O:151:ALA:N	2.81	0.44
2:O:26:ILE:HG23	2:O:26:ILE:O	2.18	0.44
3:P:27:ASN:ND2	3:P:209:PRO:HG2	2.32	0.44
5:R:86:ASN:HB2	5:R:99:ARG:HE	1.82	0.44
8:U:35:GLU:O	8:U:39:LEU:HG	2.17	0.44
3:C:247:SER:N	3:C:248:PRO:HD3	2.33	0.44
5:E:191:ASP:O	5:E:192:LEU:HD23	2.18	0.44
2:O:152:PHE:HA	2:O:157:VAL:CG1	2.47	0.44
2:O:182:ARG:NH1	2:O:182:ARG:HG2	2.32	0.44
2:O:402:ILE:O	2:O:405:VAL:HG23	2.18	0.44
8:U:18:THR:O	8:U:22:GLU:HG3	2.17	0.44
1:A:106:MET:HE3	1:A:110:VAL:HG23	1.99	0.44
2:B:150:VAL:CG2	2:B:151:ALA:N	2.80	0.44
4:D:151:PRO:HA	4:D:156:GLN:HG3	1.98	0.44
4:D:83:ARG:HH12	4:D:86:LYS:HG3	1.81	0.44
2:O:42:SER:O	2:O:113:ARG:HD2	2.17	0.44
2:O:156:GLN:HE22	9:V:75:ARG:C	2.21	0.44
3:P:325:LEU:HD21	3:P:366:LEU:HB3	1.99	0.44
3:P:50:LEU:HD23	12:P:501:HEM:HBC1	1.99	0.44
4:Q:139:ALA:HB3	8:U:54:CYS:SG	2.57	0.44
5:E:166:ASP:OD2	5:E:172:ARG:HD3	2.17	0.44
1:N:106:MET:CG	1:N:203:ILE:HD13	2.40	0.44
2:O:62:ASN:O	2:O:65:THR:CG2	2.62	0.44
2:B:424:MET:HG2	2:B:425:ALA:N	2.33	0.44
1:N:22:GLY:O	1:N:193:PRO:HA	2.18	0.44
2:O:370:MET:C	2:O:372:VAL:H	2.21	0.44
2:O:76:THR:HG23	2:O:82:SER:HB2	2.00	0.44
1:A:106:MET:HE2	1:A:107:PRO:CA	2.48	0.43
2:B:182:ARG:HH11	2:B:182:ARG:HG2	1.83	0.43
3:C:92:PHE:O	3:C:95:ILE:HG22	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:190:ASP:C	5:E:192:LEU:N	2.71	0.43
2:O:206:LEU:O	2:O:206:LEU:HG	2.17	0.43
5:R:118:ARG:NH1	5:R:171:ILE:HG13	2.33	0.43
2:B:422:LYS:O	2:B:436:LEU:HD21	2.18	0.43
4:D:209:LEU:HD23	4:D:209:LEU:HA	1.89	0.43
1:A:61:HIS:CE1	1:A:134:ILE:HG12	2.53	0.43
2:B:26:ILE:O	2:B:26:ILE:HG12	2.18	0.43
2:B:399:ALA:HA	2:B:402:ILE:HG22	1.99	0.43
3:C:278:ALA:HB1	3:C:295:LEU:CD1	2.48	0.43
5:E:185:TYR:HB3	5:E:195:VAL:HA	1.99	0.43
8:H:28:GLU:O	8:H:32:LYS:HG3	2.18	0.43
1:N:354:VAL:HG23	1:N:355:LYS:N	2.33	0.43
4:Q:166:ASN:ND2	4:Q:166:ASN:H	2.14	0.43
1:A:436:ARG:HD2	1:A:436:ARG:HA	1.89	0.43
2:B:258:VAL:HG21	2:B:321:LEU:HD22	2.00	0.43
2:B:24:LEU:HD12	2:B:37:SER:O	2.19	0.43
4:D:102:ARG:HG2	4:D:102:ARG:HH11	1.83	0.43
3:P:285:ILE:HD12	3:P:294:ALA:HB2	2.00	0.43
5:R:164:HIS:CD2	5:R:173:LYS:HD3	2.54	0.43
5:R:75:GLU:HB3	5:R:194:VAL:HG22	1.99	0.43
2:O:315:ASN:ND2	9:V:7:ARG:HD3	2.27	0.43
1:A:23:LEU:HA	1:A:192:ALA:O	2.19	0.43
2:B:101:THR:OG1	2:B:104:LYS:HG3	2.18	0.43
2:B:291:VAL:C	2:B:293:SER:H	2.22	0.43
2:O:315:ASN:HD21	9:V:7:ARG:NH1	2.16	0.43
1:A:331:ILE:HG21	1:A:431:LEU:HB2	2.01	0.43
1:A:7:THR:HG21	2:B:113:ARG:CD	2.48	0.43
8:H:49:HIS:O	8:H:50:THR:HB	2.18	0.43
1:N:398:ARG:HG2	1:N:398:ARG:HH11	1.84	0.43
1:N:430:GLN:HG2	1:N:430:GLN:O	2.19	0.43
3:P:247:SER:N	3:P:248:PRO:HD3	2.33	0.43
6:S:31:LEU:HD21	6:S:65:ALA:HB2	1.99	0.43
1:A:111:GLU:HG3	1:A:215:HIS:CD2	2.54	0.43
1:A:205:HIS:O	1:A:209:VAL:HG12	2.19	0.43
2:B:59:THR:HG22	2:B:60:THR:HG22	2.01	0.43
3:C:9:HIS:CD2	3:C:11:LEU:H	2.36	0.43
4:D:221:TYR:HD2	5:E:39:VAL:HG11	1.84	0.43
1:N:130:GLU:O	1:N:134:ILE:HG13	2.19	0.43
1:N:304:CYS:HB2	1:N:325:VAL:O	2.19	0.43
2:O:29:LEU:HB3	2:O:30:PRO:HD2	2.01	0.43
2:O:424:MET:HG2	2:O:425:ALA:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:14:HIS:CG	4:Q:21:LEU:HD23	2.54	0.43
8:U:65:ARG:O	8:U:69:VAL:HG23	2.19	0.43
10:W:52:TRP:O	10:W:56:LYS:HB2	2.18	0.43
1:A:317:THR:HG23	1:A:318:GLY:N	2.34	0.43
1:A:351:GLU:HA	1:A:354:VAL:HG22	2.01	0.43
1:A:395:TRP:CE3	1:A:398:ARG:HD2	2.54	0.43
2:B:38:LEU:CD1	2:B:39:GLU:H	2.32	0.43
5:E:83:GLU:O	5:E:85:LYS:N	2.43	0.43
2:O:46:ARG:HD2	2:O:110:GLU:CD	2.38	0.43
3:P:365:ILE:HG22	3:P:366:LEU:HD23	2.01	0.43
5:R:166:ASP:OD2	5:R:170:ARG:HB2	2.19	0.43
5:R:186:GLN:O	5:R:193:VAL:HG23	2.19	0.43
3:C:6:ARG:O	3:C:13:LYS:HA	2.19	0.43
3:C:50:LEU:O	3:C:54:MET:HG3	2.19	0.43
2:O:230:ALA:O	2:O:231:GLY:C	2.56	0.43
2:O:341:MET:HE3	2:O:417:PHE:HE2	1.79	0.43
2:O:47:ILE:HD11	2:O:116:VAL:HG13	2.01	0.43
2:O:59:THR:HG22	2:O:60:THR:HG22	1.99	0.43
3:P:344:VAL:O	3:P:345:GLU:HG3	2.18	0.43
5:R:104:ALA:HA	5:R:107:ASN:HD22	1.83	0.43
1:A:63:ALA:O	1:A:116:VAL:HG13	2.19	0.43
2:B:128:THR:HG21	2:B:224:LEU:CD2	2.49	0.43
3:C:198:LEU:HD21	12:C:502:HEM:HMA3	2.00	0.43
3:P:345:GLU:O	3:P:348:PHE:HB2	2.18	0.43
3:P:9:HIS:ND1	3:P:12:LEU:HD12	2.34	0.43
10:W:15:ARG:CG	10:W:15:ARG:HH11	2.31	0.43
2:B:31:ASN:H	2:B:31:ASN:ND2	2.16	0.42
2:B:372:VAL:O	2:B:372:VAL:HG12	2.19	0.42
3:C:347:PRO:O	3:C:350:ILE:HG22	2.18	0.42
5:E:101:ARG:HB2	5:E:131:GLU:HA	2.00	0.42
8:H:27:THR:O	8:H:31:VAL:HG23	2.19	0.42
2:O:152:PHE:HA	2:O:157:VAL:HG11	2.01	0.42
2:O:268:GLU:O	2:O:268:GLU:HG2	2.18	0.42
2:O:33:LEU:HD22	2:O:224:LEU:HD12	2.01	0.42
2:O:72:ALA:C	2:O:74:PRO:HD2	2.39	0.42
9:V:47:LEU:HD11	9:V:56:ARG:NH1	2.34	0.42
5:E:125:ASP:C	5:E:126:ARG:HG3	2.39	0.42
1:N:106:MET:HE3	1:N:110:VAL:CG2	2.49	0.42
1:N:191:LYS:O	1:N:195:MET:HG3	2.19	0.42
2:O:28:LYS:HE3	2:O:32:GLY:HA2	2.01	0.42
2:O:374:THR:HG22	2:O:376:GLN:N	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:63:LEU:HB2	2:O:182:ARG:CD	2.47	0.42
5:R:78:LEU:HD22	5:R:132:TRP:CE2	2.54	0.42
8:U:48:SER:O	8:U:49:HIS:HB2	2.18	0.42
2:B:305:GLN:HB3	2:B:306:PRO:HD2	2.00	0.42
2:B:253:VAL:O	2:B:327:ILE:HA	2.20	0.42
3:C:79:LEU:HD22	4:D:204:MET:HE3	2.01	0.42
6:F:32:MET:CE	6:F:87:LYS:HG2	2.42	0.42
7:G:72:LYS:HE2	8:H:57:GLU:OE1	2.19	0.42
1:N:119:ASN:O	1:N:120:CYS:C	2.57	0.42
1:N:219:VAL:CG1	1:N:220:SER:N	2.82	0.42
1:N:358:LYS:HE3	1:N:399:ILE:O	2.19	0.42
2:B:435:PHE:CZ	2:O:169:LYS:HG2	2.54	0.42
5:R:153:PHE:C	5:R:155:GLY:H	2.22	0.42
3:P:215:ASP:HB3	7:T:8:ALA:HB2	2.01	0.42
2:B:28:LYS:HG2	2:B:28:LYS:O	2.18	0.42
2:B:71:LEU:CD1	2:B:144:LEU:HD23	2.49	0.42
2:O:291:VAL:C	2:O:293:SER:H	2.22	0.42
2:O:368:TYR:O	2:O:372:VAL:HG23	2.20	0.42
3:P:2:ALA:CB	3:P:8:SER:HB3	2.41	0.42
4:Q:117:VAL:HG21	4:Q:191:ARG:HA	2.02	0.42
6:S:17:ARG:HG2	6:S:17:ARG:HH11	1.82	0.42
1:A:443:TRP:CE3	1:A:443:TRP:CA	3.00	0.42
2:B:341:MET:HE3	2:B:417:PHE:CE2	2.55	0.42
5:E:114:VAL:HG11	5:E:117:LEU:HD12	2.01	0.42
5:E:153:PHE:C	5:E:155:GLY:H	2.23	0.42
1:N:289:HIS:CD2	2:O:83:PHE:HD1	2.37	0.42
2:O:86:THR:O	2:O:90:GLU:HG3	2.20	0.42
3:P:9:HIS:CD2	3:P:11:LEU:H	2.37	0.42
1:N:436:ARG:NH1	3:P:220:PRO:HB2	2.34	0.42
6:S:31:LEU:HD21	6:S:65:ALA:CB	2.50	0.42
9:V:75:ARG:HD2	9:V:75:ARG:N	2.34	0.42
10:W:20:PHE:O	10:W:24:VAL:HG23	2.20	0.42
3:C:151:PHE:HB2	3:C:162:VAL:HG22	2.00	0.42
4:D:44:ASP:OD1	4:D:93:LYS:HE3	2.20	0.42
1:N:40:TRP:HZ3	1:N:376:CYS:HG	1.60	0.42
2:O:399:ALA:C	2:O:402:ILE:HG22	2.39	0.42
3:P:349:ILE:O	3:P:353:GLN:HG3	2.19	0.42
4:Q:235:MET:CE	6:S:64:ARG:HA	2.49	0.42
6:S:77:LYS:HB3	6:S:77:LYS:HE2	1.69	0.42
1:A:49:ASN:HD21	1:A:51:LYS:H	1.68	0.42
2:B:305:GLN:HB3	2:B:306:PRO:CD	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:62:LYS:O	4:D:66:GLU:HG3	2.19	0.42
5:E:81:ILE:HB	5:E:132:TRP:HH2	1.84	0.42
3:P:23:PRO:HG2	7:T:3:HIS:HB2	2.00	0.42
3:P:305:ILE:HB	3:P:306:PRO:HD3	2.02	0.42
4:Q:134:TYR:CD2	4:Q:162:PRO:HG3	2.54	0.42
1:A:37:VAL:HG12	1:A:199:ALA:HB1	2.01	0.42
3:C:130:VAL:HG23	3:C:131:GLY:N	2.34	0.42
4:D:76:GLU:OE1	4:D:76:GLU:N	2.43	0.42
4:D:232:SER:CB	7:G:23:GLN:HE22	2.32	0.42
1:N:269:VAL:HG21	1:N:410:VAL:HG21	2.02	0.42
2:O:259:THR:CG2	2:O:260:GLU:N	2.82	0.42
3:P:31:TRP:CH2	15:P:506:CDL:H512	2.55	0.42
4:D:75:ASP:O	4:Q:99:GLU:HG2	2.20	0.42
8:U:51:GLU:O	8:U:52:GLU:O	2.38	0.42
1:A:119:ASN:O	1:A:120:CYS:C	2.58	0.42
2:B:133:ARG:HA	2:B:134:PRO:HD3	1.93	0.42
2:B:73:SER:N	2:B:74:PRO:HD2	2.34	0.42
3:C:156:TYR:C	3:C:158:GLY:N	2.73	0.42
3:C:158:GLY:C	3:C:160:THR:N	2.73	0.42
2:O:372:VAL:O	2:O:372:VAL:HG12	2.20	0.42
2:O:374:THR:HG22	2:O:376:GLN:HB3	2.01	0.42
3:P:184:PHE:O	3:P:184:PHE:HD2	2.03	0.42
5:R:134:ILE:HD12	5:R:185:TYR:CD1	2.55	0.42
9:V:4:VAL:HG12	9:V:61:ASP:OD2	2.19	0.42
2:O:315:ASN:ND2	9:V:7:ARG:HH11	2.18	0.42
1:A:114:ALA:HB2	1:A:216:PHE:CE2	2.55	0.42
2:B:215:ASP:O	2:B:219:VAL:HG23	2.20	0.42
4:D:169:LEU:HD23	4:D:169:LEU:O	2.20	0.42
5:E:116:LYS:H	5:E:116:LYS:CD	2.14	0.42
5:E:76:ILE:HB	5:E:193:VAL:CG1	2.50	0.42
7:G:41:PHE:CE2	7:G:45:VAL:HG21	2.55	0.42
1:N:382:HIS:HB3	1:N:388:ARG:O	2.20	0.42
5:R:79:SER:C	5:R:81:ILE:H	2.22	0.42
2:B:128:THR:HG21	2:B:224:LEU:HD22	2.01	0.41
4:D:57:THR:HG22	4:D:58:GLU:N	2.34	0.41
9:I:49:LEU:HD11	9:I:58:ARG:NH1	2.35	0.41
10:J:15:ARG:NH1	10:J:15:ARG:HG2	2.30	0.41
1:N:217:SER:O	1:N:218:GLY:C	2.59	0.41
1:N:405:ARG:HG2	1:N:405:ARG:NH1	2.35	0.41
1:N:87:ASN:OD1	2:O:286:LYS:HD2	2.20	0.41
2:O:151:ALA:O	2:O:157:VAL:HG11	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:227:ARG:O	2:O:228:SER:O	2.38	0.41
2:O:274:VAL:O	2:O:278:VAL:HG23	2.20	0.41
3:P:286:PRO:O	3:P:287:ASN:HB2	2.20	0.41
3:P:69:HIS:HD2	3:P:73:ASN:HD22	1.63	0.41
2:B:370:MET:C	2:B:372:VAL:H	2.23	0.41
2:B:62:ASN:O	2:B:65:THR:CG2	2.63	0.41
3:C:98:HIS:CD2	12:C:502:HEM:NC	2.87	0.41
4:D:14:HIS:CG	4:D:21:LEU:HD23	2.54	0.41
5:E:126:ARG:O	5:E:127:VAL:HG23	2.19	0.41
5:E:146:PRO:HG2	5:E:180:LEU:HD21	2.01	0.41
1:N:170:THR:HG22	1:N:171:THR:H	1.84	0.41
4:Q:110:PRO:HA	4:Q:111:PRO:HD2	1.93	0.41
5:R:148:ALA:O	5:R:150:SER:N	2.53	0.41
1:A:304:CYS:HB2	1:A:325:VAL:O	2.20	0.41
2:B:57:TYR:CD1	2:B:57:TYR:N	2.87	0.41
3:C:13:LYS:HG3	3:C:17:ASN:ND2	2.36	0.41
18:D:501:HEC:HMD1	18:D:501:HEC:HAD1	1.94	0.41
1:N:35:CYS:HA	1:N:372:THR:HG21	2.02	0.41
2:O:207:VAL:HG12	2:O:208:GLY:H	1.86	0.41
12:P:501:HEM:HBC2	12:P:501:HEM:HMC1	2.02	0.41
4:Q:142:VAL:O	4:Q:142:VAL:HG23	2.19	0.41
5:R:134:ILE:HB	5:R:185:TYR:CE2	2.54	0.41
1:A:430:GLN:HG2	1:A:430:GLN:O	2.19	0.41
3:C:30:ALA:HB1	15:C:505:CDL:H111	2.02	0.41
1:N:45:SER:OG	1:N:92:ARG:HG2	2.20	0.41
2:O:59:THR:HG22	2:O:60:THR:H	1.83	0.41
2:O:96:LEU:HB3	9:V:68:LEU:CD2	2.41	0.41
4:Q:211:ILE:HG12	10:W:35:PHE:CZ	2.55	0.41
5:R:112:VAL:HG11	5:R:170:ARG:NH2	2.35	0.41
5:R:134:ILE:HD12	5:R:185:TYR:CE1	2.55	0.41
1:A:106:MET:HE3	1:A:110:VAL:CG2	2.50	0.41
2:B:166:ALA:HB1	2:B:242:GLY:C	2.40	0.41
3:C:38:LEU:HD23	3:C:38:LEU:HA	1.83	0.41
4:D:16:GLY:CA	4:D:19:SER:OG	2.68	0.41
5:E:106:ILE:O	5:E:106:ILE:HG22	2.21	0.41
5:E:164:HIS:CD2	5:E:173:LYS:HD3	2.56	0.41
10:J:58:LYS:HB2	10:J:59:TYR:CE1	2.55	0.41
1:N:106:MET:CE	1:N:110:VAL:HG21	2.50	0.41
1:N:87:ASN:CG	1:N:88:GLY:N	2.73	0.41
2:O:80:ALA:HA	2:O:84:ARG:NH1	2.25	0.41
3:P:2:ALA:HA	3:P:3:PRO:HD2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:506:CDL:HA32	7:T:40:ARG:HB3	2.03	0.41
5:R:137:GLY:O	5:R:145:VAL:HG13	2.21	0.41
5:R:83:GLU:HA	5:R:100:HIS:O	2.20	0.41
2:B:29:LEU:HB3	2:B:30:PRO:CD	2.49	0.41
3:C:51:LEU:HD23	3:C:51:LEU:HA	1.92	0.41
5:R:170:ARG:HG2	5:R:179:ASN:ND2	2.36	0.41
1:A:280:TYR:CG	1:A:281:ASP:N	2.88	0.41
3:C:285:ILE:HD12	3:C:294:ALA:HB2	2.03	0.41
4:D:68:VAL:HG11	4:D:92:PRO:CG	2.50	0.41
1:N:156:THR:CG2	1:N:157:ALA:N	2.83	0.41
1:N:350:THR:HG22	1:N:351:GLU:N	2.35	0.41
1:N:351:GLU:HA	1:N:354:VAL:HG22	2.02	0.41
2:O:22:GLU:HG3	2:O:23:ASP:N	2.30	0.41
4:Q:220:TYR:CE2	15:Q:502:CDL:H722	2.55	0.41
5:R:193:VAL:O	5:R:193:VAL:HG13	2.21	0.41
5:R:77:LYS:HG3	5:R:191:ASP:OD2	2.20	0.41
1:A:106:MET:HG3	1:A:203:ILE:HG21	2.02	0.41
5:E:170:ARG:HA	5:E:179:ASN:HB3	2.02	0.41
1:N:106:MET:HE2	1:N:107:PRO:CA	2.50	0.41
2:O:144:LEU:HB2	2:O:183:ILE:HD12	2.03	0.41
2:O:248:ASN:HD22	2:O:249:GLY:N	2.18	0.41
5:R:144:CYS:HB2	5:R:158:CYS:SG	2.61	0.41
7:T:41:PHE:CE2	7:T:45:VAL:HG21	2.56	0.41
8:U:67:HIS:CE1	8:U:71:HIS:HE1	2.38	0.41
10:W:4:ALA:O	10:W:8:GLN:HG3	2.21	0.41
2:B:374:THR:HG22	2:B:376:GLN:N	2.35	0.41
3:C:285:ILE:O	3:C:285:ILE:HG22	2.19	0.41
3:C:377:MET:HE1	6:F:20:TYR:CD1	2.56	0.41
5:E:134:ILE:CD1	5:E:193:VAL:HG21	2.50	0.41
1:N:212:ALA:O	1:N:216:PHE:HB2	2.21	0.41
1:N:45:SER:OG	1:N:92:ARG:HA	2.21	0.41
2:O:101:THR:OG1	2:O:104:LYS:HG3	2.20	0.41
3:P:186:LEU:HA	3:P:186:LEU:HD23	1.89	0.41
1:A:388:ARG:HG3	1:A:388:ARG:HH21	1.86	0.41
2:B:75:LEU:HD22	2:B:136:GLU:HB3	2.02	0.41
4:D:117:VAL:HG21	4:D:191:ARG:HA	2.03	0.41
5:E:128:LYS:O	5:E:129:LYS:C	2.58	0.41
8:H:17:LEU:HD13	8:H:73:LEU:HD22	2.01	0.41
1:N:331:ILE:HG21	1:N:431:LEU:HB2	2.03	0.41
2:O:133:ARG:HD3	2:O:135:TRP:CZ2	2.55	0.41
3:P:101:ARG:CD	3:P:101:ARG:C	2.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:19:LEU:C	3:P:20:ILE:HG13	2.41	0.41
4:Q:240:PRO:O	4:Q:241:LYS:C	2.58	0.41
5:R:112:VAL:HG11	5:R:170:ARG:HH12	1.83	0.41
8:U:51:GLU:O	8:U:52:GLU:C	2.58	0.41
2:B:26:ILE:CD1	2:B:391:THR:HA	2.48	0.41
1:A:156:THR:HA	5:E:7:VAL:HG21	2.02	0.41
1:N:144:ASP:OD1	1:N:144:ASP:C	2.59	0.41
2:O:133:ARG:HA	2:O:134:PRO:HD3	1.92	0.41
1:A:109:VAL:HA	1:A:112:LEU:HD12	2.03	0.40
4:D:116:ILE:HG23	4:D:117:VAL:N	2.36	0.40
3:C:23:PRO:HG3	7:G:4:PHE:CD1	2.55	0.40
2:O:141:GLN:N	2:O:142:PRO:HD2	2.36	0.40
2:O:200:THR:OG1	2:O:203:ARG:HD3	2.20	0.40
2:O:230:ALA:O	2:O:231:GLY:O	2.39	0.40
3:P:109:LEU:HA	3:P:109:LEU:HD23	1.81	0.40
4:Q:70:VAL:HG21	4:Q:83:ARG:CZ	2.52	0.40
6:S:87:LYS:HA	6:S:87:LYS:HD3	1.93	0.40
1:A:197:LEU:HD13	1:A:216:PHE:CE1	2.57	0.40
2:B:133:ARG:HD3	2:B:135:TRP:CZ2	2.56	0.40
5:E:131:GLU:H	5:E:131:GLU:CD	2.23	0.40
7:T:57:LEU:O	7:T:58:LEU:C	2.59	0.40
1:A:144:ASP:C	1:A:144:ASP:OD1	2.60	0.40
1:A:217:SER:O	1:A:218:GLY:C	2.60	0.40
1:A:45:SER:OG	1:A:92:ARG:HA	2.22	0.40
2:B:166:ALA:HA	2:B:240:TRP:CZ3	2.56	0.40
2:B:374:THR:HG22	2:B:376:GLN:HB3	2.02	0.40
3:P:342:GLN:NE2	3:P:342:GLN:HA	2.36	0.40
1:A:371:GLY:O	1:A:375:VAL:HG23	2.21	0.40
1:A:433:ASP:OD2	1:A:435:ASN:HB2	2.21	0.40
5:E:86:ASN:HD22	5:E:148:ALA:CB	2.33	0.40
10:J:15:ARG:CG	10:J:15:ARG:HH11	2.30	0.40
1:N:156:THR:HG23	1:N:157:ALA:N	2.37	0.40
3:P:271:PRO:HB2	3:P:275:PHE:HB2	2.03	0.40
3:P:356:SER:O	3:P:359:TYR:HB3	2.21	0.40
14:P:505:UQ:C8	14:P:505:UQ:HM51	2.51	0.40
5:R:78:LEU:N	5:R:191:ASP:O	2.48	0.40
6:S:71:LYS:O	6:S:72:HIS:HB2	2.22	0.40
4:D:214:LEU:O	4:D:218:LEU:HG	2.21	0.40
5:E:78:LEU:HD11	5:E:187:PHE:CD2	2.57	0.40
9:I:65:VAL:HG12	9:I:66:ALA:H	1.85	0.40
1:N:82:MET:CE	1:N:105:ASP:HB3	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:239:PRO:C	4:Q:241:LYS:H	2.25	0.40
7:T:24:ARG:O	7:T:27:PRO:HD3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	441/446 (99%)	408 (92%)	25 (6%)	8 (2%)	10	25
1	N	440/446 (99%)	409 (93%)	24 (6%)	7 (2%)	11	28
2	B	419/441 (95%)	351 (84%)	52 (12%)	16 (4%)	4	8
2	O	420/441 (95%)	359 (86%)	46 (11%)	15 (4%)	4	9
3	C	378/380 (100%)	350 (93%)	24 (6%)	4 (1%)	17	40
3	P	377/380 (99%)	348 (92%)	23 (6%)	6 (2%)	11	28
4	D	239/241 (99%)	222 (93%)	16 (7%)	1 (0%)	38	66
4	Q	239/241 (99%)	221 (92%)	15 (6%)	3 (1%)	14	35
5	E	194/196 (99%)	147 (76%)	31 (16%)	16 (8%)	1	1
5	R	194/196 (99%)	151 (78%)	32 (16%)	11 (6%)	2	3
6	F	99/110 (90%)	95 (96%)	4 (4%)	0	100	100
6	S	99/110 (90%)	92 (93%)	7 (7%)	0	100	100
7	G	78/81 (96%)	65 (83%)	11 (14%)	2 (3%)	6	15
7	T	77/81 (95%)	66 (86%)	9 (12%)	2 (3%)	6	15
8	H	68/77 (88%)	63 (93%)	4 (6%)	1 (2%)	12	30
8	U	65/77 (84%)	55 (85%)	8 (12%)	2 (3%)	5	11
9	I	34/76 (45%)	24 (71%)	6 (18%)	4 (12%)	0	0
9	V	34/76 (45%)	24 (71%)	6 (18%)	4 (12%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	J	59/61 (97%)	54 (92%)	5 (8%)	0	100	100
10	W	58/61 (95%)	52 (90%)	4 (7%)	2 (3%)	4	10
All	All	4012/4218 (95%)	3556 (89%)	352 (9%)	104 (3%)	6	15

All (104) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	218	GLY
1	A	433	ASP
2	B	26	ILE
2	B	39	GLU
2	B	226	ILE
3	C	287	ASN
5	E	102	THR
5	E	149	ASN
5	E	150	SER
1	N	433	ASP
2	O	19	PRO
2	O	26	ILE
2	O	39	GLU
2	O	228	SER
3	P	287	ASN
5	R	124	LEU
5	R	125	ASP
8	U	52	GLU
10	W	61	ALA
1	A	262	TRP
2	B	171	ALA
2	B	201	SER
2	B	227	ARG
2	B	228	SER
2	B	231	GLY
2	B	236	LYS
2	B	371	SER
5	E	118	ARG
5	E	163	SER
5	E	190	ASP
9	I	7	ARG
9	I	60	ALA
9	I	63	ASP
1	N	218	GLY

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Mol	Chain	Res	Type
1	N	262	TRP
1	N	282	ARG
2	O	171	ALA
2	O	201	SER
2	O	220	ALA
2	O	231	GLY
2	O	371	SER
5	R	127	VAL
5	R	163	SER
9	V	58	ALA
9	V	70	ALA
1	A	217	SER
1	A	282	ARG
2	B	29	LEU
3	C	159	HIS
5	E	84	GLY
5	E	115	SER
5	E	120	PRO
5	E	137	GLY
2	O	236	LYS
3	P	155	PRO
3	P	160	THR
5	R	149	ASN
7	T	33	ALA
9	V	7	ARG
9	V	60	ARG
1	A	71	PRO
1	A	72	CYS
2	B	221	GLU
3	C	5	ILE
5	E	112	VAL
7	G	33	ALA
1	N	81	SER
2	O	222	GLN
3	P	5	ILE
3	P	156	TYR
5	R	123	ASP
5	R	137	GLY
1	A	388	ARG
2	B	269	ALA
2	B	270	ASN
2	B	390	GLY

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Mol	Chain	Res	Type
3	C	156	TYR
5	E	186	GLN
7	G	7	LEU
8	H	50	THR
9	I	62	ARG
1	N	71	PRO
1	N	72	CYS
2	O	390	GLY
4	Q	162	PRO
5	R	108	GLN
7	T	7	LEU
8	U	27	THR
10	W	15	ARG
4	D	162	PRO
5	E	130	PRO
2	O	226	ILE
2	O	436	LEU
3	P	158	GLY
4	Q	198	HIS
5	R	130	PRO
5	R	159	PRO
4	Q	176	PRO
5	R	114	VAL
5	E	159	PRO
2	O	351	GLY
2	B	351	GLY
5	E	155	GLY
5	E	175	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	365/368 (99%)	353 (97%)	12 (3%)	43	73
1	N	365/368 (99%)	351 (96%)	14 (4%)	38	68
2	B	332/347 (96%)	317 (96%)	15 (4%)	32	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	O	333/347 (96%)	320 (96%)	13 (4%)	37	68
3	C	328/328 (100%)	318 (97%)	10 (3%)	46	76
3	P	328/328 (100%)	318 (97%)	10 (3%)	46	76
4	D	200/200 (100%)	198 (99%)	2 (1%)	80	93
4	Q	200/200 (100%)	198 (99%)	2 (1%)	80	93
5	E	166/166 (100%)	158 (95%)	8 (5%)	30	59
5	R	165/166 (99%)	161 (98%)	4 (2%)	54	83
6	F	93/96 (97%)	91 (98%)	2 (2%)	57	84
6	S	93/96 (97%)	91 (98%)	2 (2%)	57	84
7	G	71/71 (100%)	69 (97%)	2 (3%)	49	79
7	T	70/71 (99%)	68 (97%)	2 (3%)	48	77
8	H	65/71 (92%)	64 (98%)	1 (2%)	70	90
8	U	63/71 (89%)	63 (100%)	0	100	100
9	I	26/45 (58%)	25 (96%)	1 (4%)	38	68
9	V	26/45 (58%)	26 (100%)	0	100	100
10	J	49/49 (100%)	47 (96%)	2 (4%)	35	66
10	W	47/49 (96%)	44 (94%)	3 (6%)	20	45
All	All	3385/3482 (97%)	3280 (97%)	105 (3%)	45	75

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	A	58	PHE
1	A	86	PHE
1	A	102	LEU
1	A	106	MET
1	A	226	ASP
1	A	281	ASP
1	A	342	TRP
1	A	395	TRP
1	A	405	ARG
1	A	432	LEU
1	A	443	TRP
2	B	31	ASN
2	B	97	SER

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Mol	Chain	Res	Type
2	B	104	LYS
2	B	114	ASP
2	B	117	ASP
2	B	124	LEU
2	B	154	SER
2	B	170	THR
2	B	181	TYR
2	B	248	ASN
2	B	250	HIS
2	B	325	TYR
2	B	335	GLU
2	B	341	MET
2	B	402	ILE
3	C	21	ASP
3	C	81	ARG
3	C	82	ASN
3	C	91	PHE
3	C	157	ILE
3	C	184	PHE
3	C	223	PRO
3	C	226	SER
3	C	240	PHE
3	C	256	ASN
4	D	169	LEU
4	D	203	ARG
5	E	31	ASP
5	E	107	ASN
5	E	116	LYS
5	E	123	ASP
5	E	131	GLU
5	E	149	ASN
5	E	186	GLN
5	E	191	ASP
6	F	64	ARG
6	F	70	LEU
7	G	27	PRO
7	G	79	ASN
8	H	49	HIS
9	I	71	ASN
10	J	59	TYR
10	J	60	GLU
1	N	3	THR

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Mol	Chain	Res	Type
1	N	18	THR
1	N	49	ASN
1	N	58	PHE
1	N	86	PHE
1	N	102	LEU
1	N	106	MET
1	N	281	ASP
1	N	308	GLN
1	N	342	TRP
1	N	395	TRP
1	N	405	ARG
1	N	432	LEU
1	N	443	TRP
2	O	19	PRO
2	O	31	ASN
2	O	104	LYS
2	O	114	ASP
2	O	117	ASP
2	O	154	SER
2	O	181	TYR
2	O	248	ASN
2	O	250	HIS
2	O	325	TYR
2	O	335	GLU
2	O	341	MET
2	O	402	ILE
3	P	21	ASP
3	P	81	ARG
3	P	82	ASN
3	P	91	PHE
3	P	184	PHE
3	P	207	ASN
3	P	226	SER
3	P	240	PHE
3	P	256	ASN
3	P	380	TYR
4	Q	169	LEU
4	Q	203	ARG
5	R	3	ASN
5	R	31	ASP
5	R	130	PRO
5	R	190	ASP

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Mol	Chain	Res	Type
6	S	64	ARG
6	S	70	LEU
7	T	27	PRO
7	T	79	ASN
10	W	15	ARG
10	W	59	TYR
10	W	60	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	118	GLN
1	A	274	ASN
1	A	289	HIS
1	A	308	GLN
1	A	339	GLN
2	B	31	ASN
2	B	156	GLN
2	B	225	ASN
2	B	248	ASN
2	B	276	GLN
2	B	315	ASN
2	B	343	GLN
2	B	362	ASN
2	B	380	ASN
3	C	9	HIS
3	C	17	ASN
3	C	69	HIS
3	C	82	ASN
3	C	207	ASN
3	C	332	ASN
3	C	342	GLN
4	D	35	GLN
4	D	50	ASN
4	D	148	HIS
4	D	166	ASN
5	E	3	ASN
5	E	57	GLN
5	E	107	ASN
5	E	122	HIS
5	E	149	ASN
5	E	164	HIS

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Mol	Chain	Res	Type
7	G	23	GLN
7	G	44	GLN
7	G	73	ASN
7	G	79	ASN
9	I	71	ASN
1	N	118	GLN
1	N	274	ASN
1	N	289	HIS
1	N	308	GLN
1	N	339	GLN
2	O	31	ASN
2	O	156	GLN
2	O	248	ASN
2	O	276	GLN
2	O	297	GLN
2	O	315	ASN
2	O	332	HIS
2	O	343	GLN
2	O	362	ASN
2	O	380	ASN
3	P	9	HIS
3	P	17	ASN
3	P	69	HIS
3	P	82	ASN
3	P	207	ASN
3	P	332	ASN
3	P	342	GLN
4	Q	35	GLN
4	Q	50	ASN
4	Q	148	HIS
5	R	3	ASN
5	R	57	GLN
5	R	107	ASN
5	R	122	HIS
5	R	164	HIS
5	R	186	GLN
6	S	72	HIS
7	T	23	GLN
7	T	44	GLN
7	T	73	ASN
7	T	79	ASN
8	U	71	HIS

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Mol	Chain	Res	Type
9	V	69	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$
3	FME	C	1	3	8,8,10	2.02	2 (25%)	7,8,11	1.29	1 (14%)

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
3	FME	C	1	3	-	0/4/8/11	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1	FME	CN-N	-4.81	1.33	1.46
3	C	1	FME	CA-C	2.65	1.53	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	FME	CN-N-CA	2.51	121.79	113.60

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

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 31 ligands modelled in this entry, 2 are unknown - leaving 29 for Mogul analysis.

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	HEM	C	501	3	28,50,50	1.89	6 (21%)	17,82,82	1.72	4 (23%)
12	HEM	C	502	3	28,50,50	1.89	8 (28%)	17,82,82	1.98	4 (23%)
13	WF3	C	503	-	32,33,33	2.78	14 (43%)	39,47,47	2.36	13 (33%)
14	UQ	C	504	-	19,19,63	2.51	9 (47%)	23,26,79	1.01	1 (4%)
15	CDL	C	505	-	41,41,99	1.19	2 (4%)	43,53,111	1.11	5 (11%)
16	PEE	C	506	-	48,48,50	1.28	7 (14%)	50,53,55	0.89	4 (8%)
16	PEE	C	507	-	20,20,50	1.76	7 (35%)	22,25,55	0.64	0
17	GOL	C	508	-	5,5,5	1.38	0	5,5,5	0.67	0
18	HEC	D	501	4	28,50,50	2.05	6 (21%)	16,82,82	1.55	4 (25%)
19	BOG	D	502	-	20,20,20	0.88	0	25,25,25	0.86	1 (4%)
19	BOG	D	503	-	13,13,20	1.41	3 (23%)	18,18,25	1.17	2 (11%)
20	FES	E	501	5	0,4,4	0.00	-	0,4,4	0.00	-
16	PEE	E	502	-	49,49,50	1.45	10 (20%)	51,54,55	1.02	5 (9%)
15	CDL	G	101	-	39,39,99	1.20	2 (5%)	41,51,111	1.17	4 (9%)
16	PEE	N	502	-	4,4,50	3.49	4 (100%)	6,6,55	0.50	0
12	HEM	P	501	3	28,50,50	1.88	6 (21%)	17,82,82	1.56	4 (23%)
12	HEM	P	502	3	28,50,50	1.85	6 (21%)	17,82,82	1.77	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	BOG	P	503	-	12,12,20	1.49	3 (25%)	17,17,25	0.54	0
13	WF3	P	504	-	32,33,33	2.92	14 (43%)	39,47,47	2.37	13 (33%)
14	UQ	P	505	-	19,19,63	2.49	10 (52%)	23,26,79	0.99	1 (4%)
15	CDL	P	506	-	39,39,99	1.22	2 (5%)	41,51,111	1.18	4 (9%)
16	PEE	P	507	-	48,48,50	1.26	6 (12%)	50,53,55	0.87	4 (8%)
17	GOL	P	508	-	5,5,5	1.41	1 (20%)	5,5,5	0.67	0
18	HEC	Q	501	4	28,50,50	1.81	2 (7%)	16,82,82	1.58	4 (25%)
15	CDL	Q	502	-	41,41,99	1.19	1 (2%)	43,53,111	1.12	5 (11%)
19	BOG	Q	503	-	20,20,20	0.96	2 (10%)	25,25,25	0.88	1 (4%)
19	BOG	Q	504	-	13,13,20	1.32	2 (15%)	18,18,25	1.09	2 (11%)
20	FES	R	501	5	0,4,4	0.00	-	0,4,4	0.00	-
16	PEE	R	502	-	47,47,50	1.36	8 (17%)	48,51,55	0.77	1 (2%)

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	HEM	C	501	3	-	0/6/54/54	0/0/8/8
12	HEM	C	502	3	-	0/6/54/54	0/0/8/8
13	WF3	C	503	-	-	0/24/24/24	0/3/3/3
14	UQ	C	504	-	-	0/11/35/87	0/1/1/1
15	CDL	C	505	-	-	0/51/51/110	0/0/0/0
16	PEE	C	506	-	-	0/52/52/54	0/0/0/0
16	PEE	C	507	-	-	0/24/24/54	0/0/0/0
17	GOL	C	508	-	-	0/4/4/4	0/0/0/0
18	HEC	D	501	4	-	0/6/54/54	0/0/8/8
19	BOG	D	502	-	-	0/11/31/31	0/1/1/1
19	BOG	D	503	-	-	0/4/24/31	0/1/1/1
20	FES	E	501	5	-	0/0/4/4	0/1/1/1
16	PEE	E	502	-	-	0/53/53/54	0/0/0/0
15	CDL	G	101	-	-	0/49/49/110	0/0/0/0
16	PEE	N	502	-	-	0/0/0/54	0/0/0/0
12	HEM	P	501	3	-	0/6/54/54	0/0/8/8
12	HEM	P	502	3	-	0/6/54/54	0/0/8/8
19	BOG	P	503	-	-	0/2/22/31	0/1/1/1
13	WF3	P	504	-	-	0/24/24/24	0/3/3/3
14	UQ	P	505	-	-	0/11/35/87	0/1/1/1
15	CDL	P	506	-	-	0/49/49/110	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	PEE	P	507	-	-	0/52/52/54	0/0/0/0
17	GOL	P	508	-	-	0/4/4/4	0/0/0/0
18	HEC	Q	501	4	-	0/6/54/54	0/0/8/8
15	CDL	Q	502	-	-	0/51/51/110	0/0/0/0
19	BOG	Q	503	-	-	0/11/31/31	0/1/1/1
19	BOG	Q	504	-	-	0/4/24/31	0/1/1/1
20	FES	R	501	5	-	0/0/4/4	0/1/1/1
16	PEE	R	502	-	-	0/49/49/54	0/0/0/0

All (141) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	Q	501	HEC	C3B-C2B	-6.43	1.34	1.40
18	D	501	HEC	C3C-C2C	-6.13	1.34	1.40
13	P	504	WF3	C9-C5	-5.67	1.42	1.49
18	D	501	HEC	C3B-C2B	-5.43	1.35	1.40
18	Q	501	HEC	C3C-C2C	-5.38	1.35	1.40
13	C	503	WF3	C9-C5	-5.10	1.42	1.49
12	C	501	HEM	C3B-CAB	-4.57	1.38	1.47
12	P	502	HEM	C3B-CAB	-4.41	1.39	1.47
12	C	502	HEM	C3B-CAB	-4.41	1.39	1.47
12	P	501	HEM	C3B-CAB	-4.32	1.39	1.47
12	C	501	HEM	C3C-CAC	-4.29	1.39	1.47
12	P	501	HEM	C3C-CAC	-4.25	1.39	1.47
13	P	504	WF3	C15-C14	-3.84	1.40	1.50
13	C	503	WF3	C15-C14	-3.72	1.40	1.50
12	P	502	HEM	C3C-CAC	-3.61	1.40	1.47
12	C	502	HEM	C3C-C2C	-3.46	1.35	1.40
12	C	502	HEM	C3B-C2B	-3.28	1.36	1.40
12	P	502	HEM	C3B-C2B	-3.24	1.36	1.40
16	P	507	PEE	C19-C18	-3.05	1.34	1.51
12	P	501	HEM	C3B-C2B	-3.04	1.36	1.40
16	C	506	PEE	C19-C18	-3.01	1.34	1.51
16	P	507	PEE	C22-C21	-3.01	1.34	1.51
16	C	506	PEE	C22-C21	-2.85	1.35	1.51
12	C	501	HEM	C3C-C2C	-2.80	1.36	1.40
16	E	502	PEE	C19-C18	-2.79	1.35	1.51
16	E	502	PEE	C22-C21	-2.76	1.35	1.51
12	P	501	HEM	C3C-C2C	-2.42	1.37	1.40
12	C	502	HEM	C3C-CAC	-2.30	1.43	1.47
16	R	502	PEE	C19-C18	-2.30	1.35	1.51
18	D	501	HEC	C1D-CHD	-2.26	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	C	506	PEE	C31-C30	2.01	1.56	1.50
16	E	502	PEE	O2-C2	2.03	1.51	1.46
17	P	508	GOL	O2-C2	2.03	1.49	1.43
15	G	101	CDL	O1-C1	2.04	1.49	1.43
19	D	503	BOG	C1-C2	2.04	1.58	1.52
16	C	507	PEE	P-O4P	2.06	1.67	1.59
13	C	503	WF3	C11-C12	2.06	1.43	1.38
16	N	502	PEE	P-O2P	2.07	1.61	1.54
13	P	504	WF3	C28-C26	2.09	1.44	1.38
12	C	502	HEM	C4D-ND	2.10	1.39	1.36
15	C	505	CDL	OA6-CA5	2.13	1.40	1.34
19	Q	503	BOG	O5-C1	2.14	1.47	1.41
15	G	101	CDL	CB3-CB4	2.16	1.56	1.50
19	Q	503	BOG	C4-C5	2.18	1.57	1.53
16	C	507	PEE	C3-C2	2.19	1.56	1.50
13	C	503	WF3	C11-C10	2.20	1.43	1.38
16	P	507	PEE	C3-C2	2.20	1.57	1.50
16	R	502	PEE	C31-C30	2.21	1.57	1.50
16	E	502	PEE	C31-C30	2.21	1.57	1.50
19	P	503	BOG	C1-C2	2.22	1.57	1.52
16	C	507	PEE	C11-C10	2.23	1.57	1.50
13	C	503	WF3	C28-C26	2.24	1.45	1.38
16	C	506	PEE	C3-C2	2.28	1.57	1.50
15	P	506	CDL	O1-C1	2.29	1.50	1.43
13	P	504	WF3	C11-C12	2.29	1.43	1.38
14	P	505	UQ	C7-C8	2.32	1.54	1.50
15	P	506	CDL	CB3-CB4	2.32	1.57	1.50
19	Q	504	BOG	C4-C5	2.33	1.58	1.53
19	P	503	BOG	C4-C5	2.35	1.58	1.53
19	D	503	BOG	O5-C1	2.35	1.47	1.41
12	P	502	HEM	C1B-NB	2.38	1.39	1.36
14	C	504	UQ	O2-C2	2.40	1.42	1.36
16	R	502	PEE	C1-C2	2.41	1.57	1.50
19	Q	504	BOG	O5-C1	2.42	1.47	1.41
12	C	501	HEM	C1B-NB	2.42	1.39	1.36
16	R	502	PEE	C3-C2	2.43	1.57	1.50
13	P	504	WF3	C11-C10	2.43	1.43	1.38
14	P	505	UQ	C5-C4	2.43	1.56	1.47
14	C	504	UQ	C5-C4	2.44	1.56	1.47
15	Q	502	CDL	O1-C1	2.44	1.50	1.43
18	D	501	HEC	C3B-C4B	2.48	1.47	1.43
16	E	502	PEE	C11-C10	2.48	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	P	505	UQ	C3-C4	2.49	1.56	1.48
13	C	503	WF3	C19-C18	2.53	1.55	1.51
15	C	505	CDL	O1-C1	2.55	1.51	1.43
16	R	502	PEE	C11-C10	2.56	1.58	1.50
14	P	505	UQ	O2-C2	2.57	1.43	1.36
13	C	503	WF3	C13-C14	2.61	1.44	1.39
19	D	503	BOG	C4-C5	2.64	1.58	1.53
16	P	507	PEE	P-O1P	2.64	1.60	1.50
14	C	504	UQ	C3-C4	2.64	1.56	1.48
18	D	501	HEC	C4A-NA	2.65	1.39	1.36
16	C	506	PEE	O2-C10	2.65	1.42	1.34
14	C	504	UQ	CM5-C5	2.66	1.56	1.50
18	D	501	HEC	C4B-NB	2.66	1.39	1.36
14	P	505	UQ	CM5-C5	2.67	1.56	1.50
13	P	504	WF3	C19-C18	2.69	1.55	1.51
16	C	507	PEE	C1-C2	2.69	1.58	1.50
16	C	506	PEE	P-O1P	2.71	1.61	1.50
16	E	502	PEE	C1-C2	2.71	1.58	1.50
16	N	502	PEE	P-O3P	2.71	1.64	1.54
16	E	502	PEE	C3-C2	2.71	1.58	1.50
13	P	504	WF3	C25-C26	2.76	1.43	1.37
16	P	507	PEE	O2-C10	2.77	1.42	1.34
13	P	504	WF3	C10-C9	2.80	1.44	1.39
19	P	503	BOG	O5-C1	2.80	1.48	1.43
16	C	507	PEE	O3-C30	2.81	1.41	1.33
14	P	505	UQ	C2-C1	2.81	1.57	1.48
12	P	502	HEM	CBB-CAB	2.88	1.49	1.28
16	R	502	PEE	P-O1P	2.89	1.61	1.50
16	C	507	PEE	P-O1P	2.90	1.61	1.50
16	N	502	PEE	P-O4P	2.91	1.64	1.54
16	C	507	PEE	O2-C10	2.95	1.42	1.34
14	C	504	UQ	C2-C1	2.96	1.57	1.48
13	C	503	WF3	C17-N31	3.03	1.37	1.30
12	C	502	HEM	C1B-NB	3.04	1.40	1.36
16	E	502	PEE	P-O1P	3.06	1.62	1.50
16	P	507	PEE	O3-C30	3.08	1.42	1.33
14	C	504	UQ	O3-C3	3.09	1.44	1.36
14	P	505	UQ	O3-C3	3.12	1.44	1.36
13	P	504	WF3	C13-C14	3.17	1.45	1.39
16	R	502	PEE	O3-C30	3.18	1.42	1.33
16	E	502	PEE	O3-C30	3.19	1.42	1.33
13	C	503	WF3	C25-C26	3.19	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	C	503	WF3	C10-C9	3.19	1.45	1.39
13	C	503	WF3	C29-C28	3.22	1.43	1.36
13	P	504	WF3	C17-N31	3.22	1.38	1.30
16	R	502	PEE	O2-C10	3.23	1.43	1.34
12	C	502	HEM	CBB-CAB	3.23	1.51	1.28
12	C	501	HEM	CBB-CAB	3.25	1.51	1.28
13	P	504	WF3	C29-C28	3.31	1.43	1.36
16	C	506	PEE	O3-C30	3.33	1.43	1.33
12	P	501	HEM	CBB-CAB	3.37	1.52	1.28
12	C	502	HEM	CBC-CAC	3.42	1.52	1.28
16	E	502	PEE	O2-C10	3.47	1.44	1.34
12	P	502	HEM	CBC-CAC	3.56	1.54	1.28
12	C	501	HEM	CBC-CAC	3.58	1.54	1.28
12	P	501	HEM	CBC-CAC	3.58	1.54	1.28
14	P	505	UQ	C6-C1	3.76	1.57	1.46
14	P	505	UQ	C6-C5	3.91	1.43	1.35
14	C	504	UQ	C6-C5	4.01	1.44	1.35
14	C	504	UQ	C6-C1	4.06	1.58	1.46
13	C	503	WF3	C9-C14	5.02	1.47	1.40
13	C	503	WF3	C18-N23	5.09	1.37	1.30
14	C	504	UQ	C7-C6	5.32	1.60	1.51
14	P	505	UQ	C7-C6	5.34	1.60	1.51
16	N	502	PEE	P-O1P	5.35	1.62	1.50
13	P	504	WF3	C9-C14	5.35	1.47	1.40
13	P	504	WF3	C18-N23	5.58	1.38	1.30
13	C	503	WF3	C6-C5	8.60	1.53	1.35
13	P	504	WF3	C6-C5	8.97	1.54	1.35

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	P	504	WF3	C8-O7-C6	-5.73	108.57	115.71
13	C	503	WF3	C8-O7-C6	-5.23	109.20	115.71
12	C	502	HEM	C4C-C3C-C2C	-5.00	103.41	106.90
13	C	503	WF3	O2-C3-O4	-3.65	116.42	123.54
13	C	503	WF3	C26-C25-C24	-3.61	118.09	121.14
13	P	504	WF3	O2-C3-O4	-3.51	116.69	123.54
15	P	506	CDL	CB4-OB6-CB5	-3.44	109.75	117.88
12	P	502	HEM	C4C-C3C-C2C	-3.37	104.54	106.90
13	P	504	WF3	C26-C25-C24	-3.34	118.32	121.14
15	G	101	CDL	CB4-OB6-CB5	-3.28	110.12	117.88
18	D	501	HEC	CAA-C2A-C3A	-3.12	120.09	129.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	Q	501	HEC	CAA-C2A-C3A	-3.03	120.36	129.00
15	P	506	CDL	CA6-CA4-CA3	-2.77	105.61	111.86
15	G	101	CDL	CA6-CA4-CA3	-2.68	105.82	111.86
13	P	504	WF3	O4-C3-C5	-2.59	117.70	124.21
13	P	504	WF3	C10-C9-C5	-2.57	115.53	119.77
12	P	501	HEM	C4A-C3A-C2A	-2.55	105.22	107.00
13	C	503	WF3	C10-C9-C5	-2.48	115.68	119.77
12	C	502	HEM	C4A-C3A-C2A	-2.48	105.27	107.00
15	C	505	CDL	CA6-CA4-CA3	-2.46	106.31	111.86
15	G	101	CDL	CA4-OA6-CA5	-2.44	112.11	117.88
12	C	502	HEM	CAD-C3D-C2D	-2.43	122.06	129.00
13	C	503	WF3	C24-C30-N31	-2.41	117.95	121.21
15	Q	502	CDL	CA6-CA4-CA3	-2.36	106.53	111.86
12	C	501	HEM	C4A-C3A-C2A	-2.35	105.36	107.00
13	C	503	WF3	O4-C3-C5	-2.33	118.35	124.21
15	C	505	CDL	CB4-OB6-CB5	-2.29	112.47	117.88
15	Q	502	CDL	CA4-OA6-CA5	-2.28	112.48	117.88
15	P	506	CDL	CA4-OA6-CA5	-2.23	112.60	117.88
15	Q	502	CDL	CB4-OB6-CB5	-2.21	112.66	117.88
15	Q	502	CDL	CA6-OA8-CA7	-2.17	111.63	117.17
15	C	505	CDL	CA6-OA8-CA7	-2.17	111.64	117.17
12	P	502	HEM	CAD-C3D-C2D	-2.15	122.86	129.00
18	D	501	HEC	CAD-C3D-C2D	-2.13	122.93	129.00
13	P	504	WF3	C28-C29-C30	-2.13	118.23	120.84
13	C	503	WF3	C28-C29-C30	-2.12	118.24	120.84
18	Q	501	HEC	CMD-C2D-C1D	-2.12	125.21	128.46
15	C	505	CDL	CA4-OA6-CA5	-2.10	112.92	117.88
13	P	504	WF3	C24-C30-N31	-2.08	118.39	121.21
15	C	505	CDL	CB6-CB4-CB3	-2.02	107.30	111.86
15	Q	502	CDL	CB6-CB4-CB3	-2.02	107.31	111.86
15	G	101	CDL	OB6-CB4-CB3	2.02	115.79	108.44
12	P	501	HEM	CMC-C2C-C3C	2.05	128.69	124.89
13	P	504	WF3	O16-C15-C14	2.08	115.30	109.24
15	P	506	CDL	OB6-CB4-CB3	2.13	116.19	108.44
13	C	503	WF3	O16-C15-C14	2.14	115.45	109.24
16	C	506	PEE	C22-C21-C20	2.23	125.93	114.45
16	P	507	PEE	C22-C21-C20	2.24	125.97	114.45
13	P	504	WF3	C28-C26-C25	2.31	121.27	118.47
16	P	507	PEE	C23-C22-C21	2.33	126.46	114.45
19	Q	504	BOG	O1-C1-C2	2.39	110.98	108.14
16	C	506	PEE	C23-C22-C21	2.42	126.90	114.45
16	R	502	PEE	O3-C3-C2	2.42	114.74	108.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	E	502	PEE	C23-C22-C21	2.42	126.94	114.45
16	P	507	PEE	C19-C18-C17	2.44	127.01	114.45
12	P	501	HEM	C3B-C4B-NB	2.44	112.36	109.21
16	C	506	PEE	C19-C18-C17	2.45	127.09	114.45
16	E	502	PEE	O3-C3-C2	2.48	114.90	108.66
16	E	502	PEE	C22-C21-C20	2.49	127.31	114.45
12	C	501	HEM	C3B-C4B-NB	2.54	112.50	109.21
18	Q	501	HEC	CBD-CAD-C3D	2.59	117.44	112.48
13	C	503	WF3	C28-C26-C25	2.64	121.67	118.47
19	D	503	BOG	O1-C1-C2	2.64	111.29	108.14
16	E	502	PEE	C19-C18-C17	2.68	128.27	114.45
18	D	501	HEC	CBD-CAD-C3D	2.71	117.66	112.48
16	E	502	PEE	C20-C19-C18	2.71	128.44	114.45
16	P	507	PEE	C20-C19-C18	2.73	128.53	114.45
16	C	506	PEE	C20-C19-C18	2.76	128.68	114.45
18	D	501	HEC	CBA-CAA-C2A	2.87	117.95	112.47
14	P	505	UQ	C8-C7-C6	2.94	120.10	111.85
19	D	502	BOG	C1'-O1-C1	2.95	118.92	113.87
14	C	504	UQ	C8-C7-C6	3.11	120.58	111.85
12	C	501	HEM	CMB-C2B-C3B	3.12	130.68	124.89
19	Q	503	BOG	C1'-O1-C1	3.20	119.36	113.87
13	P	504	WF3	C17-N31-C30	3.24	122.76	116.30
12	C	502	HEM	CBA-CAA-C2A	3.31	118.81	112.48
12	P	501	HEM	CBD-CAD-C3D	3.35	118.86	112.47
19	Q	504	BOG	C1'-O1-C1	3.36	118.53	113.29
13	C	503	WF3	C17-N31-C30	3.37	123.01	116.30
13	C	503	WF3	C18-N23-C24	3.45	122.75	115.05
13	P	504	WF3	C18-N23-C24	3.47	122.81	115.05
13	P	504	WF3	C1-O2-C3	3.60	122.70	115.87
19	D	503	BOG	C1'-O1-C1	3.61	118.93	113.29
12	C	501	HEM	CBD-CAD-C3D	3.66	119.45	112.47
18	Q	501	HEC	CBA-CAA-C2A	3.69	119.50	112.47
13	C	503	WF3	C1-O2-C3	3.75	122.97	115.87
12	P	502	HEM	CBA-CAA-C2A	3.93	119.99	112.48
13	C	503	WF3	O2-C3-C5	8.40	125.22	111.91
13	P	504	WF3	O2-C3-C5	8.64	125.61	111.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

17 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	C	501	HEM	1	0
12	C	502	HEM	4	0
13	C	503	WF3	1	0
14	C	504	UQ	3	0
15	C	505	CDL	1	0
16	C	506	PEE	2	0
18	D	501	HEC	2	0
15	G	101	CDL	1	0
12	P	501	HEM	2	0
12	P	502	HEM	2	0
13	P	504	WF3	1	0
14	P	505	UQ	2	0
15	P	506	CDL	3	0
16	P	507	PEE	2	0
18	Q	501	HEC	1	0
15	Q	502	CDL	1	0
16	R	502	PEE	1	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	443/446 (99%)	-0.12	4 (0%) 84 85	40, 70, 101, 123	0
1	N	442/446 (99%)	0.07	11 (2%) 58 58	44, 76, 104, 117	0
2	B	421/441 (95%)	0.16	12 (2%) 52 52	55, 88, 120, 147	0
2	O	422/441 (95%)	0.18	23 (5%) 26 24	49, 81, 114, 133	0
3	C	379/380 (99%)	-0.19	11 (2%) 52 52	29, 47, 92, 135	0
3	P	379/380 (99%)	-0.05	13 (3%) 46 45	37, 68, 106, 127	0
4	D	241/241 (100%)	-0.23	5 (2%) 64 65	37, 49, 89, 118	0
4	Q	241/241 (100%)	0.41	13 (5%) 26 25	51, 82, 115, 128	0
5	E	196/196 (100%)	1.36	55 (28%) 1 0	41, 118, 173, 190	0
5	R	196/196 (100%)	0.73	36 (18%) 1 1	49, 99, 152, 173	0
6	F	101/110 (91%)	-0.45	0 100 100	31, 51, 71, 100	0
6	S	101/110 (91%)	0.22	6 (5%) 23 21	60, 79, 123, 146	0
7	G	80/81 (98%)	0.09	4 (5%) 30 28	37, 62, 116, 128	0
7	T	79/81 (97%)	0.78	12 (15%) 2 2	55, 91, 150, 165	0
8	H	70/77 (90%)	-0.02	3 (4%) 36 34	45, 69, 101, 145	0
8	U	67/77 (87%)	1.20	15 (22%) 1 1	97, 129, 149, 155	0
9	I	37/76 (48%)	2.33	18 (48%) 0 0	80, 124, 163, 166	0
9	V	37/76 (48%)	2.43	21 (56%) 0 0	61, 126, 162, 163	0
10	J	61/61 (100%)	-0.09	4 (6%) 19 17	46, 65, 107, 170	0
10	W	60/61 (98%)	0.26	7 (11%) 5 4	62, 81, 128, 138	0
All	All	4053/4218 (96%)	0.20	273 (6%) 19 16	29, 74, 134, 190	0

All (273) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	E	113	ASP	12.3
8	H	9	GLU	9.0
5	E	104	ALA	7.8
5	E	108	GLN	7.6
8	U	13	LEU	7.4
9	I	3	SER	7.4
5	E	126	ARG	7.2
9	I	57	GLY	7.2
9	V	54	SER	7.2
5	E	110	ALA	7.1
5	E	157	TYR	7.0
5	E	109	GLU	7.0
5	E	114	VAL	6.9
5	E	112	VAL	6.7
5	E	102	THR	6.7
5	E	124	LEU	6.6
7	T	77	TYR	6.3
5	E	107	ASN	6.3
5	E	115	SER	6.2
9	V	2	LEU	6.1
5	E	173	LYS	6.1
5	E	103	GLN	6.0
7	T	78	GLU	6.0
7	T	74	PRO	6.0
9	V	55	GLY	5.8
5	E	120	PRO	5.7
5	E	188	VAL	5.6
2	O	19	PRO	5.6
9	V	61	ASP	5.6
10	J	64	GLU	5.5
5	E	174	GLY	5.3
9	I	51	CYS	5.3
9	I	50	LEU	5.1
9	I	6	ALA	5.1
5	E	116	LYS	5.1
5	E	127	VAL	5.0
7	T	2	ILE	5.0
8	H	10	GLU	5.0
2	O	222	GLN	4.9
5	E	149	ASN	4.9
6	S	11	ARG	4.8
5	R	186	GLN	4.8
9	I	2	LEU	4.8

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Mol	Chain	Res	Type	RSRZ
3	P	8	SER	4.8
3	C	5	ILE	4.8
9	I	48	PRO	4.7
3	C	4	ASN	4.7
6	S	12	LEU	4.7
9	V	51	GLU	4.7
3	C	8	SER	4.7
5	E	147	ILE	4.7
5	E	125	ASP	4.7
4	D	241	LYS	4.6
9	V	50	ARG	4.5
5	R	120	PRO	4.5
9	V	46	PRO	4.5
10	J	62	SER	4.5
5	R	112	VAL	4.3
3	C	7	LYS	4.3
8	U	12	GLU	4.3
9	V	48	LEU	4.3
5	E	190	ASP	4.2
10	J	63	GLU	4.2
9	I	56	SER	4.2
9	V	3	SER	4.1
9	I	63	ASP	4.1
5	E	122	HIS	4.1
7	T	75	ALA	4.1
5	R	171	ILE	4.0
2	B	350	GLY	4.0
9	I	55	MET	4.0
5	E	117	LEU	4.0
9	I	53	GLU	4.0
5	R	111	GLU	4.0
5	R	114	VAL	3.9
4	Q	241	LYS	3.9
3	C	6	ARG	3.8
3	P	156	TYR	3.8
7	T	73	ASN	3.8
7	G	2	ILE	3.7
8	U	49	HIS	3.7
2	O	18	CYS	3.7
5	E	169	GLY	3.7
9	V	53	MET	3.7
7	G	81	GLN	3.7

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Mol	Chain	Res	Type	RSRZ
5	R	102	THR	3.7
9	I	52	ARG	3.7
3	P	2	ALA	3.7
5	E	165	TYR	3.7
9	V	8	SER	3.6
3	C	2	ALA	3.6
8	U	50	THR	3.6
9	V	52	SER	3.6
5	R	157	TYR	3.6
3	P	5	ILE	3.6
3	C	156	TYR	3.6
5	E	172	ARG	3.6
5	R	196	GLY	3.5
7	T	80	ASP	3.5
5	R	167	ALA	3.5
2	B	226	ILE	3.5
5	E	86	ASN	3.5
5	R	118	ARG	3.5
5	R	188	VAL	3.5
2	O	323	GLY	3.4
5	E	159	PRO	3.4
1	N	29	GLU	3.4
5	E	121	GLN	3.4
5	E	146	PRO	3.4
9	V	59	ARG	3.3
5	R	124	LEU	3.3
3	P	4	ASN	3.3
2	O	23	ASP	3.3
5	E	79	SER	3.3
2	O	310	SER	3.3
5	R	104	ALA	3.3
6	S	13	MET	3.3
9	I	76	VAL	3.2
7	T	38	TRP	3.2
7	T	30	PHE	3.2
1	A	219	VAL	3.2
5	R	122	HIS	3.2
5	R	164	HIS	3.2
5	R	168	SER	3.2
5	E	150	SER	3.1
2	O	223	PHE	3.1
10	W	45	HIS	3.1

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Mol	Chain	Res	Type	RSRZ
5	R	125	ASP	3.1
9	I	54	SER	3.1
5	R	172	ARG	3.1
1	A	218	GLY	3.1
3	P	7	LYS	3.1
5	E	162	GLY	3.1
2	B	227	ARG	3.1
1	N	56	GLY	3.1
8	U	44	VAL	3.1
1	N	179	ARG	3.0
9	V	49	CYS	3.0
5	R	173	LYS	3.0
9	I	8	SER	3.0
5	R	113	ASP	3.0
3	P	6	ARG	3.0
9	V	5	ALA	3.0
5	E	78	LEU	2.9
1	N	227	ALA	2.9
4	Q	77	ASN	2.9
2	O	350	GLY	2.9
5	R	178	TYR	2.9
5	R	85	LYS	2.9
2	O	280	GLY	2.9
5	R	121	GLN	2.9
3	C	155	PRO	2.9
8	U	35	GLU	2.9
5	E	148	ALA	2.9
9	V	4	VAL	2.9
5	E	163	SER	2.8
9	I	7	ARG	2.8
5	R	103	GLN	2.8
6	S	10	GLY	2.8
10	W	62	SER	2.8
2	B	323	GLY	2.8
4	Q	143	VAL	2.8
5	E	167	ALA	2.8
8	U	78	LYS	2.8
7	T	66	PHE	2.7
1	N	217	SER	2.7
10	W	60	GLU	2.7
6	S	110	LYS	2.7
9	V	47	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
5	R	165	TYR	2.7
2	B	232	THR	2.7
5	E	175	PRO	2.6
2	O	304	THR	2.6
5	R	116	LYS	2.6
2	O	279	LEU	2.6
5	R	176	ALA	2.6
8	U	54	CYS	2.6
5	E	83	GLU	2.6
10	W	63	GLU	2.6
5	R	155	GLY	2.6
8	U	26	GLN	2.5
9	V	6	ALA	2.5
7	T	32	ASP	2.5
5	R	11	SER	2.5
4	Q	139	ALA	2.5
3	P	3	PRO	2.5
4	Q	187	CYS	2.5
8	U	31	VAL	2.5
9	V	74	VAL	2.5
5	E	98	VAL	2.4
5	E	106	ILE	2.4
4	D	80	LEU	2.4
5	R	117	LEU	2.4
10	W	61	ALA	2.4
4	Q	79	GLU	2.4
4	Q	25	SER	2.4
2	B	208	GLY	2.4
4	Q	82	MET	2.4
2	B	348	ALA	2.4
5	R	154	GLY	2.4
6	S	15	ARG	2.4
2	O	303	THR	2.4
5	E	158	CYS	2.4
5	E	152	ASP	2.3
5	E	171	ILE	2.3
1	A	221	PHE	2.3
5	E	85	LYS	2.3
2	B	310	SER	2.3
7	G	79	ASN	2.3
3	C	9	HIS	2.3
5	E	180	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
5	R	115	SER	2.3
7	T	46	PHE	2.3
9	V	56	ARG	2.3
4	Q	146	GLY	2.3
5	E	168	SER	2.3
8	U	32	LYS	2.3
8	U	14	VAL	2.3
9	I	77	ARG	2.3
1	N	38	GLY	2.2
1	N	432	LEU	2.2
3	P	250	LEU	2.2
2	B	41	PHE	2.2
2	O	324	PHE	2.2
2	O	106	THR	2.2
5	E	187	PHE	2.2
10	W	57	HIS	2.2
2	O	47	ILE	2.2
3	C	157	ILE	2.2
2	O	108	CYS	2.2
8	U	39	LEU	2.2
5	E	97	PHE	2.2
9	V	75	ARG	2.2
8	H	71	HIS	2.2
3	C	131	GLY	2.2
8	U	33	ALA	2.2
3	P	157	ILE	2.2
2	B	69	LEU	2.2
3	P	346	HIS	2.2
5	R	174	GLY	2.2
1	A	217	SER	2.1
4	D	145	GLU	2.1
5	R	81	ILE	2.1
2	O	277	HIS	2.1
5	E	84	GLY	2.1
2	O	312	PHE	2.1
3	P	345	GLU	2.1
2	O	400	GLN	2.1
9	I	4	VAL	2.1
2	O	386	ALA	2.1
4	Q	145	GLU	2.1
8	U	48	SER	2.1
4	D	79	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
2	O	313	ASN	2.1
4	Q	68	VAL	2.1
5	E	183	PRO	2.1
5	R	190	ASP	2.1
7	G	3	HIS	2.1
2	O	48	GLY	2.1
1	N	5	ALA	2.1
2	B	235	ALA	2.1
4	D	76	GLU	2.1
1	N	218	GLY	2.1
4	Q	165	TYR	2.0
4	Q	183	ALA	2.0
10	J	61	ALA	2.0
1	N	197	LEU	2.0
3	P	155	PRO	2.0
2	B	388	LEU	2.0
5	E	192	LEU	2.0
2	O	226	ILE	2.0
10	W	56	LYS	2.0
1	N	113	LEU	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	FME	C	1	9/11	0.64	0.62	-	139,141,148,153	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
14	UQ	P	505	19/63	0.76	0.41	8.37	80,127,140,146	0
19	BOG	P	503	12/20	0.58	0.39	7.49	126,144,149,158	0
15	CDL	Q	502	42/100	0.56	0.45	6.98	79,169,202,203	0
11	UNL	N	501	1/-	0.95	0.68	6.70	47,47,47,47	0
15	CDL	C	505	42/100	0.70	0.35	6.09	65,134,159,163	0
14	UQ	C	504	19/63	0.82	0.32	5.42	73,96,104,108	0
16	PEE	E	502	50/51	0.82	0.32	5.25	59,86,114,117	0
11	UNL	A	501	1/-	0.90	0.48	4.53	48,48,48,48	0
17	GOL	P	508	6/6	0.92	0.25	4.23	67,76,82,84	0
17	GOL	C	508	6/6	0.90	0.26	3.83	64,72,75,76	0
16	PEE	R	502	49/51	0.77	0.31	3.52	51,98,121,125	0
16	PEE	P	507	49/51	0.87	0.31	2.70	72,91,119,123	0
16	PEE	C	507	21/51	0.73	0.30	2.54	64,135,154,156	0
19	BOG	Q	503	20/20	0.91	0.27	2.09	72,100,105,113	0
15	CDL	P	506	40/100	0.83	0.27	1.94	110,125,138,141	0
16	PEE	C	506	49/51	0.92	0.23	1.94	33,60,91,103	0
15	CDL	G	101	40/100	0.92	0.21	1.46	46,83,125,131	0
12	HEM	P	501	43/43	0.98	0.22	0.92	39,58,68,81	0
12	HEM	C	502	43/43	0.98	0.21	0.91	21,39,48,59	0
12	HEM	C	501	43/43	0.98	0.21	0.81	23,41,51,66	0
13	WF3	C	503	31/31	0.97	0.17	0.37	30,40,53,60	0
13	WF3	P	504	31/31	0.96	0.18	0.24	51,64,73,78	0
12	HEM	P	502	43/43	0.99	0.17	-0.08	36,50,69,74	0
19	BOG	D	502	20/20	0.95	0.14	-0.20	44,64,72,76	0
18	HEC	Q	501	43/43	0.97	0.15	-0.39	48,60,77,85	0
18	HEC	D	501	43/43	0.99	0.12	-0.53	7,31,49,55	0
20	FES	R	501	4/4	0.99	0.08	-1.41	78,88,91,94	0
20	FES	E	501	4/4	0.97	0.08	-2.11	125,129,129,130	0
16	PEE	N	502	5/51	0.83	0.20	-	132,134,139,140	0
19	BOG	Q	504	13/20	0.54	0.50	-	179,186,190,192	0
19	BOG	D	503	13/20	0.49	0.56	-	140,156,162,164	0

6.5 Other polymers

There are no such residues in this entry.