Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:14 AM GMT

PDB ID	:	3L72
Title	:	Chicken cytochrome BC1 complex with kresoxym-I-dimethyl bound
Authors	:	Huang, L.; Zhang, Z.; Berry, E.A.
Deposited on	:	2009-12-27
Resolution	:	3.06 Å(reported)

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

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

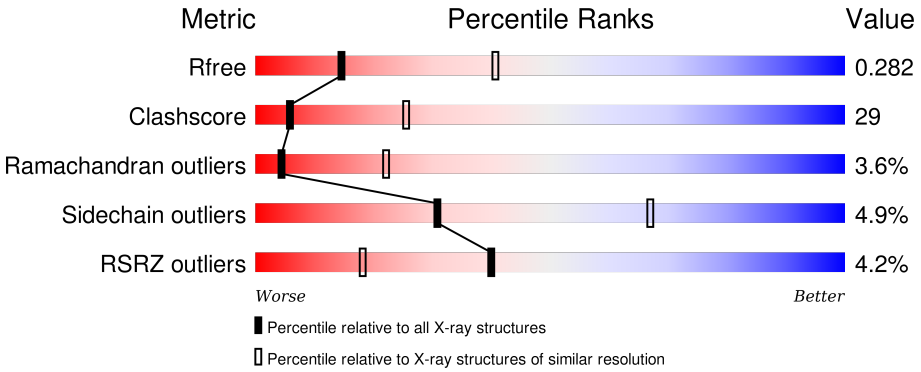
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.06 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1191 (3.10-3.02)
Clashscore	102246	1303 (3.10-3.02)
Ramachandran outliers	100387	1254 (3.10-3.02)
Sidechain outliers	100360	1254 (3.10-3.02)
RSRZ outliers	91569	1197 (3.10-3.02)

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

Mol	Chain	Length	Quality of chain
1	A	446	54% 41%
1	N	446	49% 45% 5%
2	B	441	41% 48% 6% 5%
2	O	441	44% 47% 5%
3	C	380	56% 40%

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Mol	Chain	Length	Quality of chain
3	P	380	54% 42%
4	D	241	56% 41%
4	Q	241	52% 44%
5	E	196	32% 41% 51% 9%
5	R	196	19% 45% 49% 6%
6	F	110	65% 23% 5% 8%
6	S	110	59% 28% 5% 8%
7	G	81	49% 40% 10%
7	T	81	9% 49% 42% 5%
8	H	77	48% 43% 9%
8	U	77	8% 36% 47% 13%
9	I	47	23% 40% 43% 15%
9	V	47	21% 32% 51% 9% 9%
10	J	61	61% 38%
10	W	61	54% 39% 5%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	UQ	C	2002	-	-	-	X
13	UQ	P	3002	-	-	-	X
14	CDL	D	2003	-	-	-	X
14	CDL	P	3004	-	-	-	X
14	CDL	Q	3003	-	-	-	X
15	PEE	C	2007	-	-	-	X
15	PEE	C	2008	-	-	-	X
15	PEE	E	2005	-	-	-	X
15	PEE	P	3007	-	-	-	X
15	PEE	P	3008	-	X	-	-
15	PEE	R	3005	-	-	-	X
16	GOL	C	2011	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	GOL	P	3011	-	-	-	X
18	BOG	D	2009	-	-	-	X
18	BOG	P	2010	-	-	-	X
18	BOG	Q	3009	-	-	-	X
19	FES	E	501	-	-	X	-
19	FES	R	501	-	-	X	-

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 32648 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	444	Total	C	N	O	S	0	0	0
			3447	2160	607	659	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
			3137	1970	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
			3017	2022	478	505	12			
3	P	379	Total	C	N	O	S	0	0	0
			3012	2019	477	504	12			

- 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 5, RIESKE IRONSULFUR PROTEIN, 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			

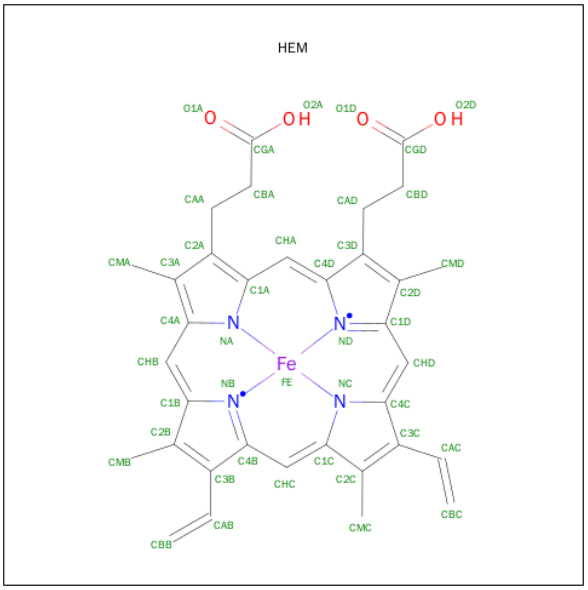
- Molecule 9 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	46	Total	C	N	O	S	0	0	0
			287	171	58	56	2			
9	V	43	Total	C	N	O	S	0	0	0
			277	167	55	53	2			

- Molecule 10 is a protein called MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 7.2 KDA PROTEIN.

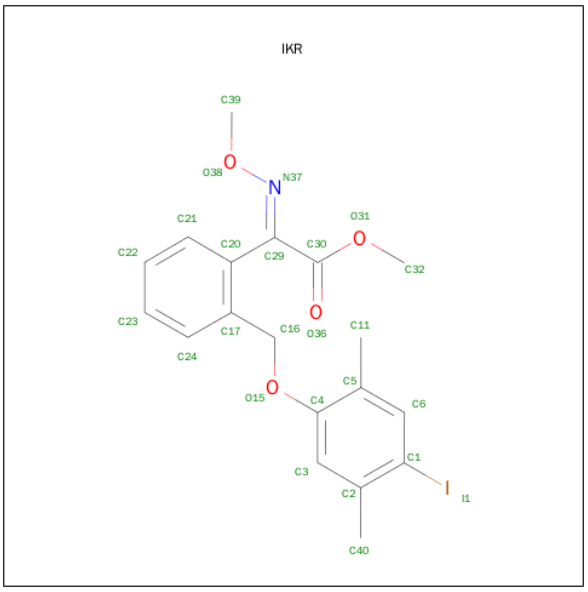
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	61	Total	C	N	O	0	0	0
			497	321	87	89			
10	W	60	Total	C	N	O	0	0	1
			479	311	86	82			

- Molecule 11 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



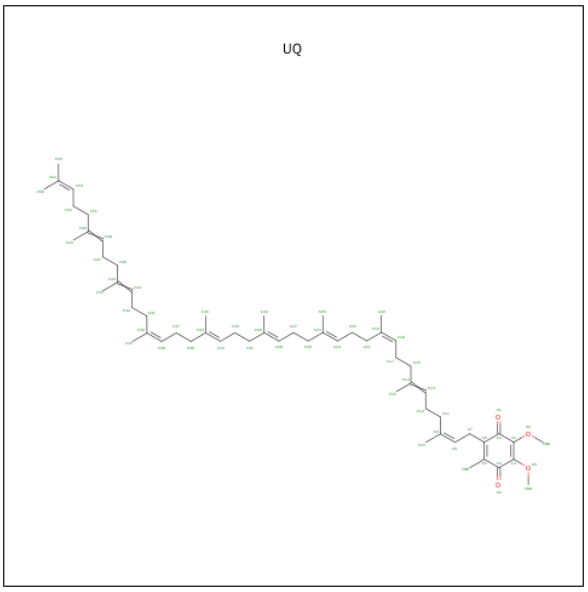
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
11	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
11	P	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
11	P	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 12 is METHYL (2E)-{2-[(4-IODO-2,5-DIMETHYLPHENOXY)METHYL]PHENYL}(METHOXYIMINO)ETHANOATE (three-letter code: IKR) (formula: $C_{19}H_{20}INO_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	C	1	Total	C	I	N	O	0	0
			25	19	1	1	4		
12	P	1	Total	C	I	N	O	0	0
			25	19	1	1	4		

- Molecule 13 is COENZYME Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-ISOMER (three-letter code: UQ) (formula: $C_{59}H_{90}O_4$).



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

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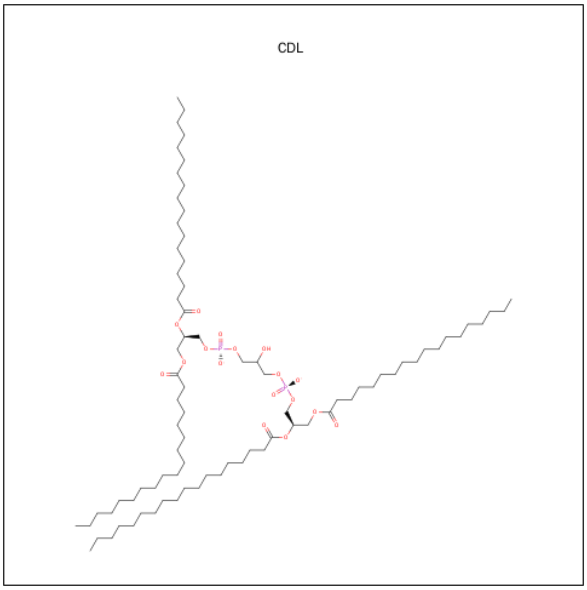
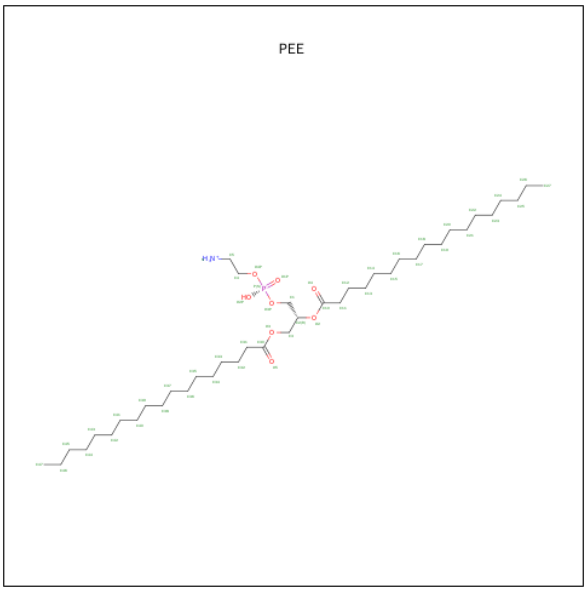
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	P	1	Total	C	O	0	0
			19	15	4		

- Molecule 14 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



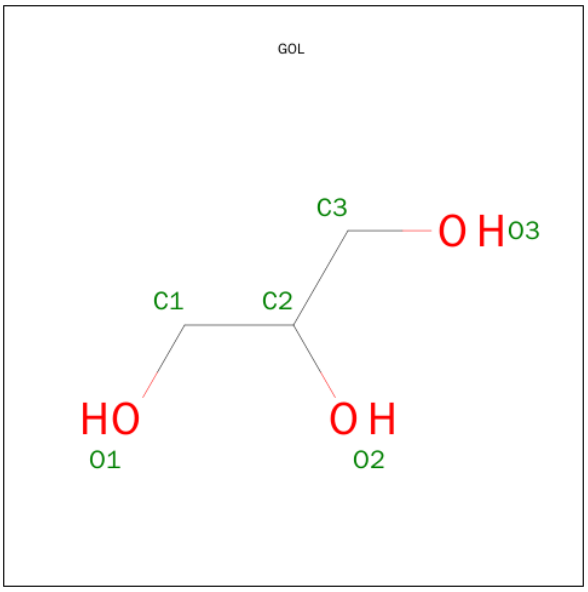
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	C	1	Total	C	O	P	0	0
			40	21	17	2		
14	D	1	Total	C	O	P	0	0
			42	23	17	2		
14	P	1	Total	C	O	P	0	0
			40	21	17	2		
14	Q	1	Total	C	O	P	0	0
			42	23	17	2		

- Molecule 15 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOETHANOLAMINE (three-letter code: PEE) (formula: $C_{41}H_{83}NO_8P$).



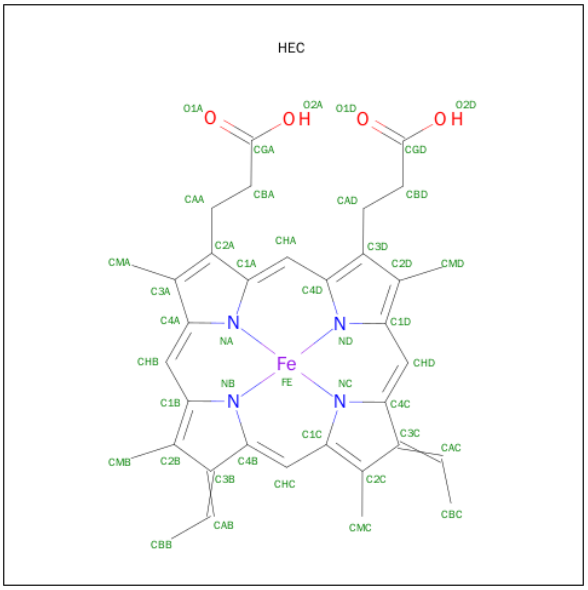
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	C	1	Total C N O P 49 39 1 8 1	0	0
15	C	1	Total C O P 21 12 8 1	0	0
15	E	1	Total C N O P 50 40 1 8 1	0	0
15	P	1	Total C N O P 49 39 1 8 1	0	0
15	P	1	Total O P 5 4 1	0	0
15	R	1	Total C N O P 50 40 1 8 1	0	0

- Molecule 16 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



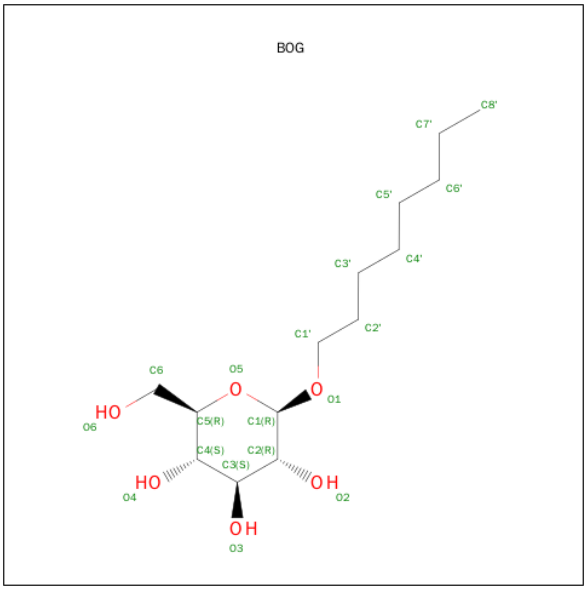
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	C	1	Total	C	O	0	0
			6	3	3		
16	P	1	Total	C	O	0	0
			6	3	3		

- Molecule 17 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



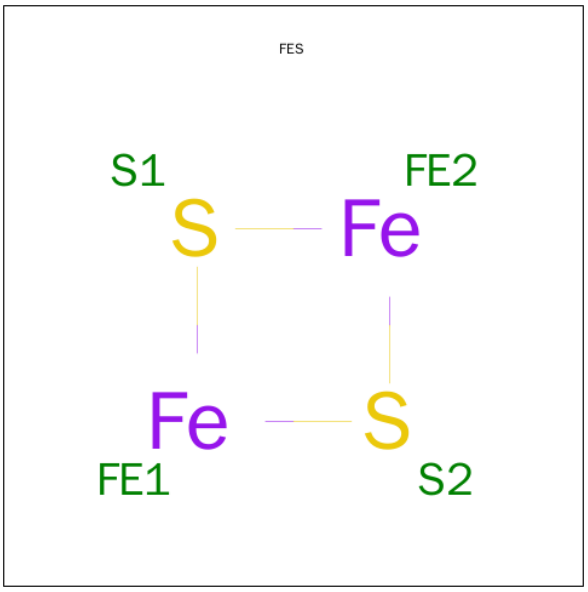
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
17	Q	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 18 is SUGAR (B-OCTYLGLUCOSIDE) (three-letter code: BOG) (formula: $C_{14}H_{28}O_6$).



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

- Molecule 19 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



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

- Molecule 20 is water.

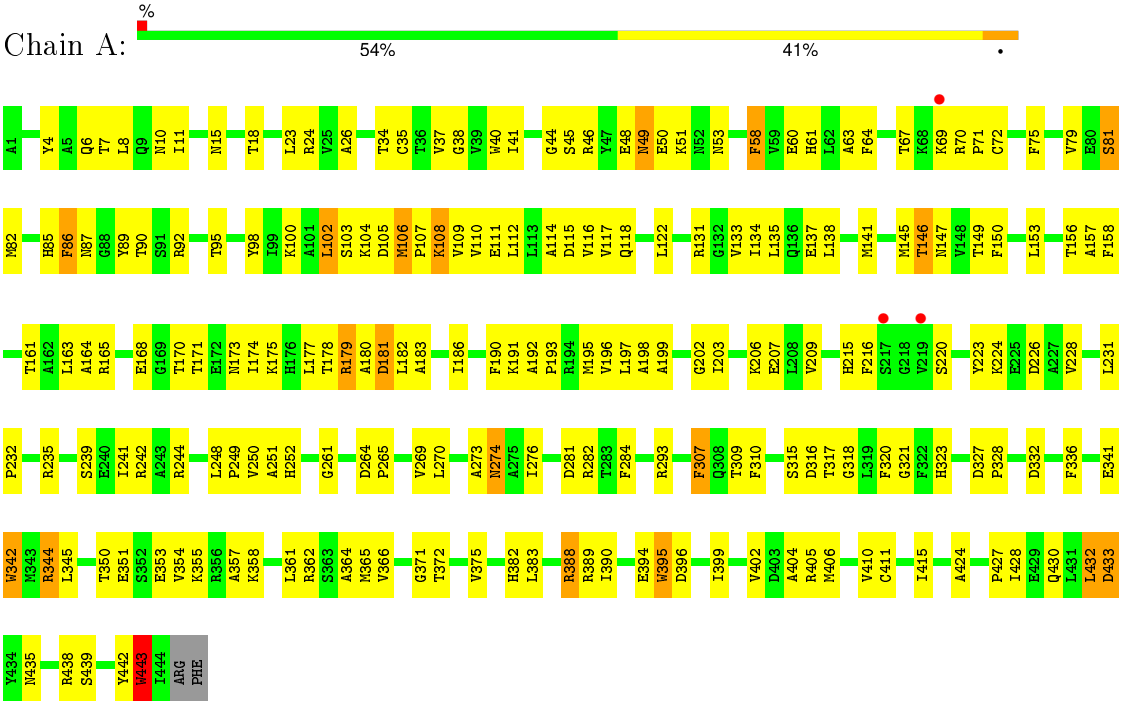
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	C	8	Total O 8 8	0	0
20	E	1	Total O 1 1	0	0
20	P	8	Total O 8 8	0	0
20	R	1	Total O 1 1	0	0

3 Residue-property plots

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

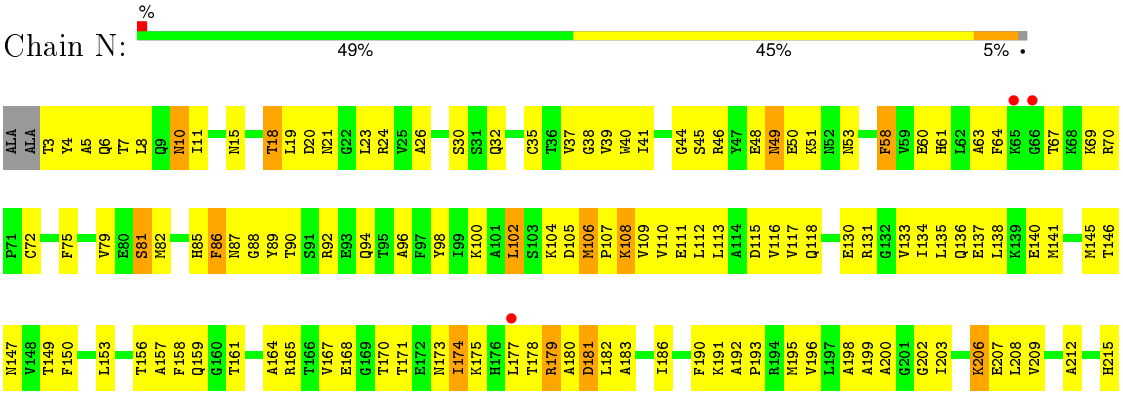
• Molecule 1: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN I

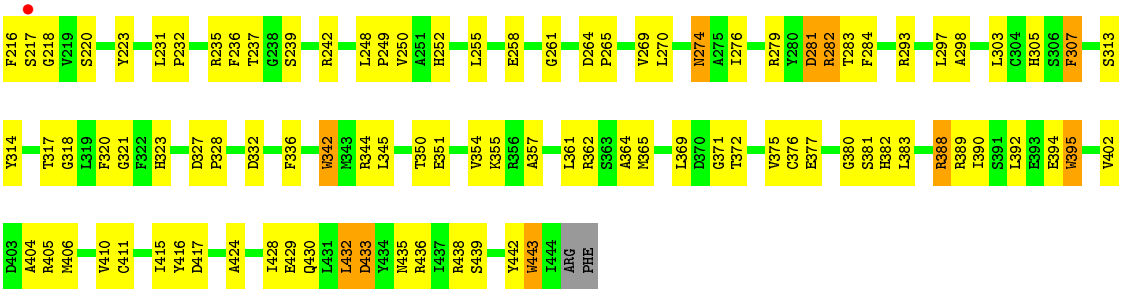
Chain A:



• Molecule 1: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN I

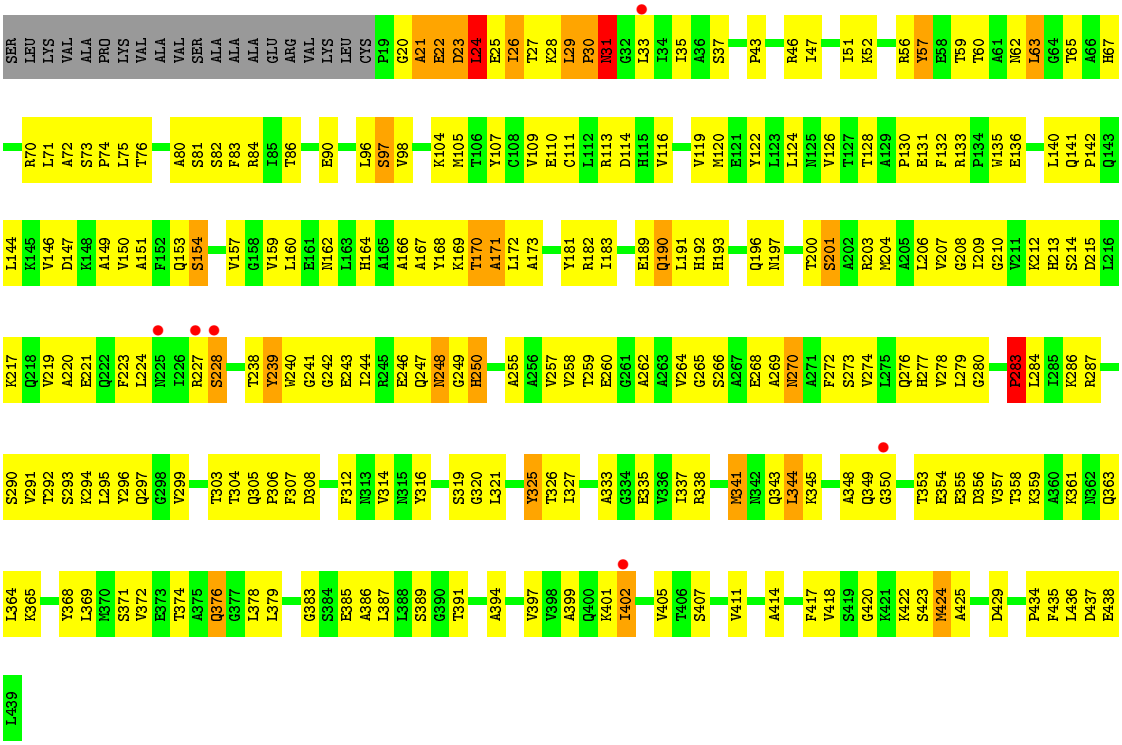
Chain N:





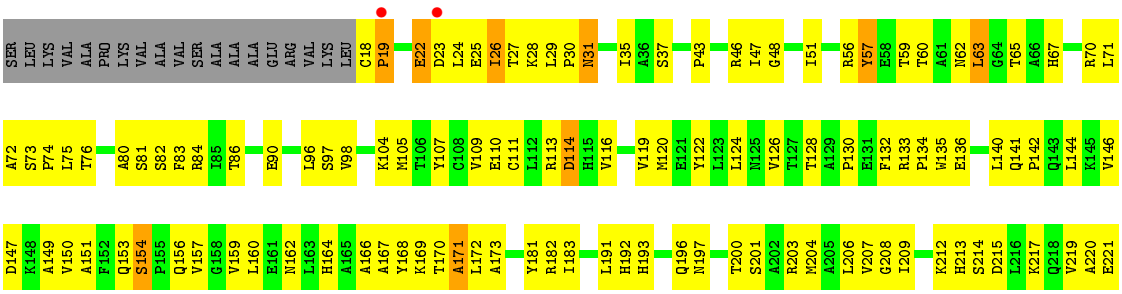
• Molecule 2: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 2

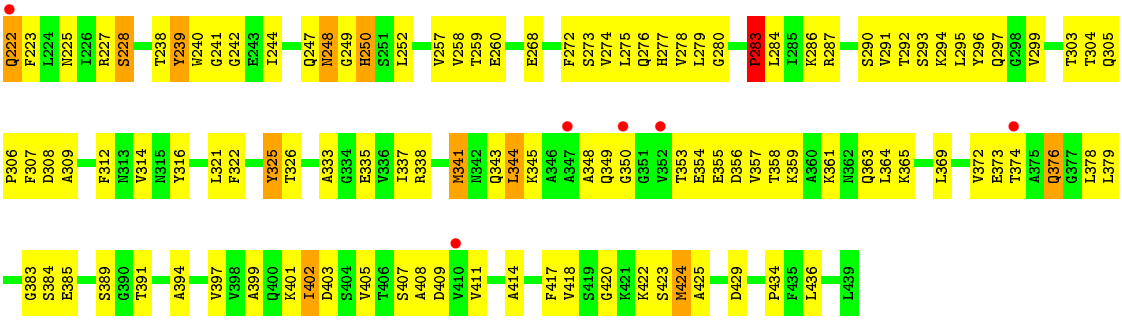
Chain B:



• Molecule 2: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 2

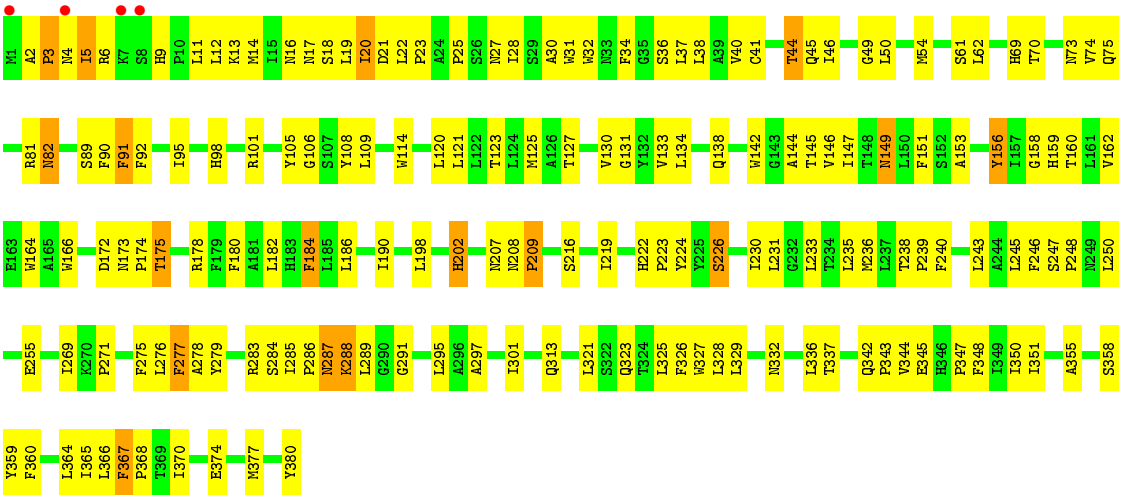
Chain O:





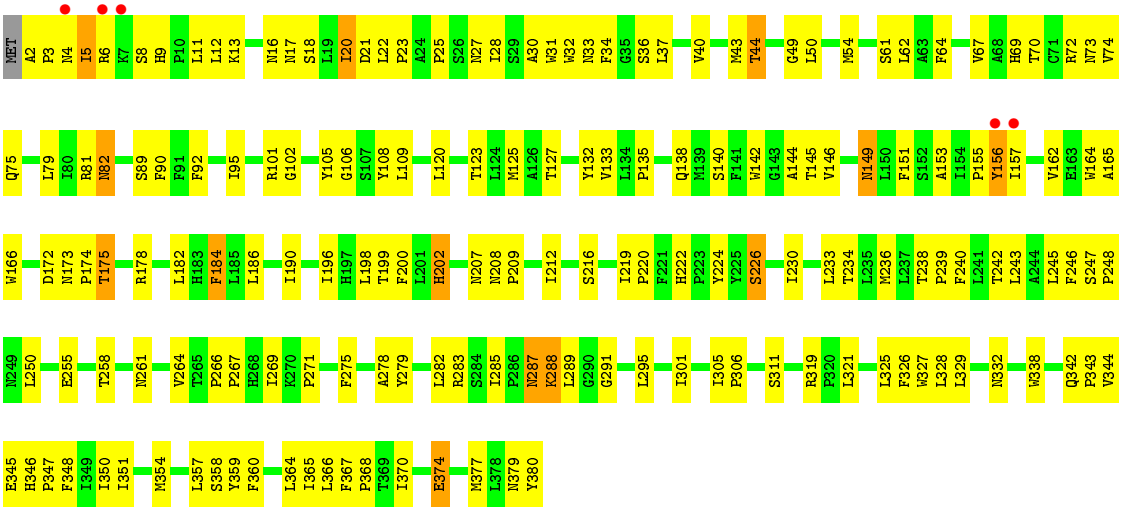
• Molecule 3: CYTOCHROME B

Chain C:



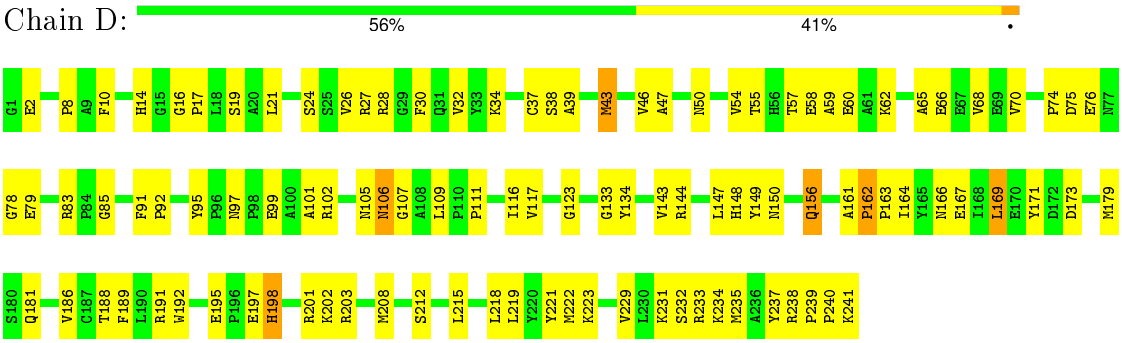
• Molecule 3: CYTOCHROME B

Chain P:



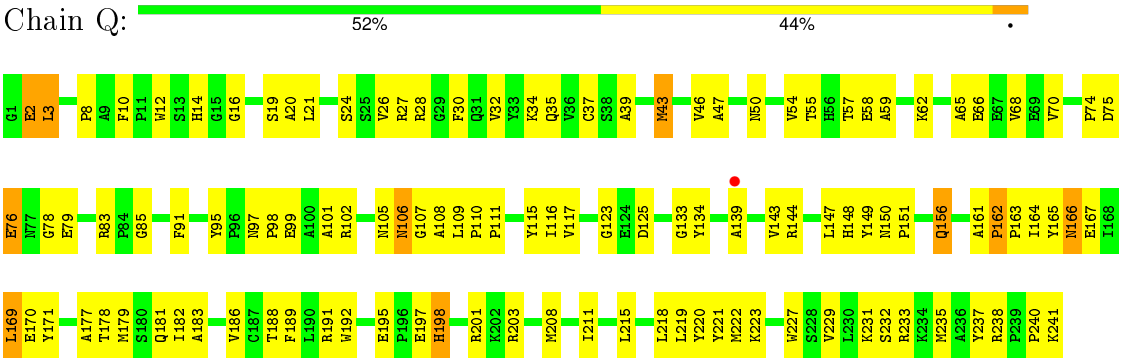
• Molecule 4: MITOCHONDRIAL CYTOCHROME C1, HEME PROTEIN

Chain D:



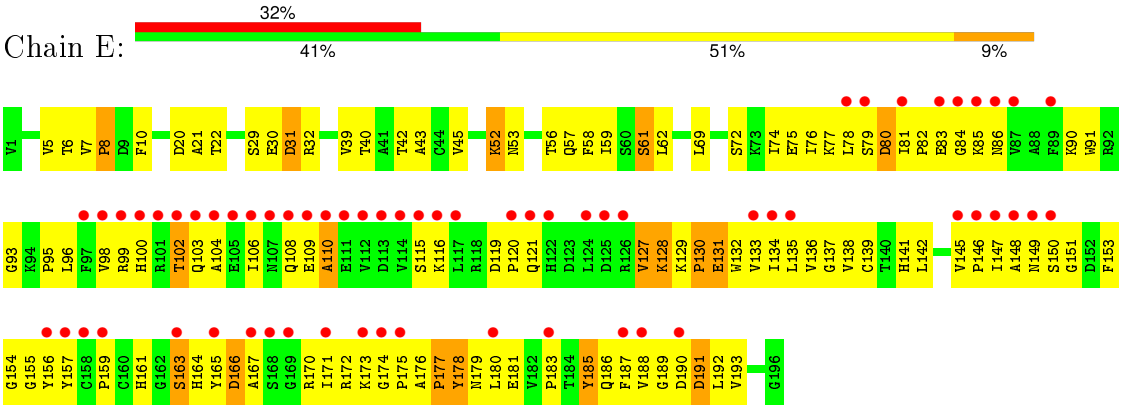
• Molecule 4: MITOCHONDRIAL CYTOCHROME C1, HEME PROTEIN

Chain Q:



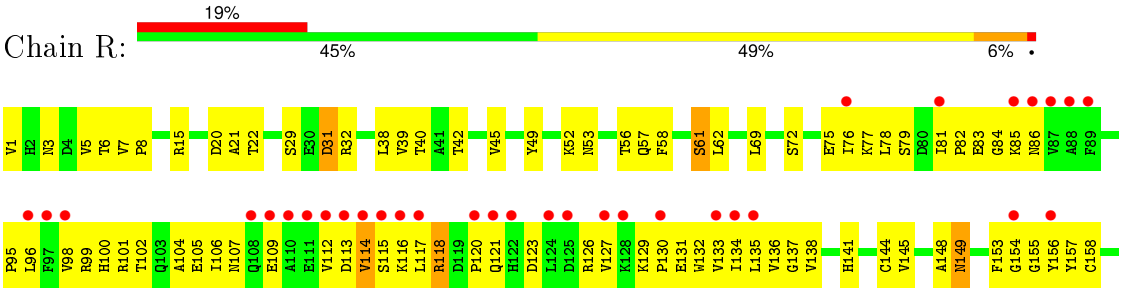
• Molecule 5: CYTOCHROME B-C1 COMPLEX SUBUNIT 5, RIESKE IRONSULFUR PROTEIN, MITOCHONDRIAL

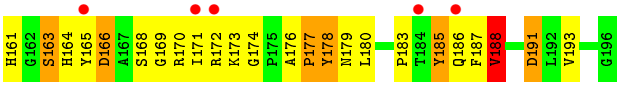
Chain E:



• Molecule 5: CYTOCHROME B-C1 COMPLEX SUBUNIT 5, RIESKE IRONSULFUR PROTEIN, MITOCHONDRIAL

Chain R:



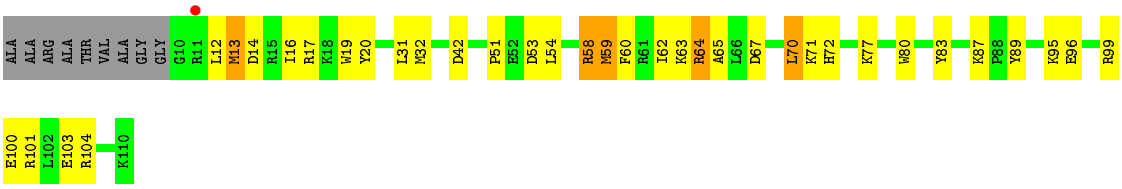


• Molecule 6: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 14 KDA PROTEIN

Chain F:

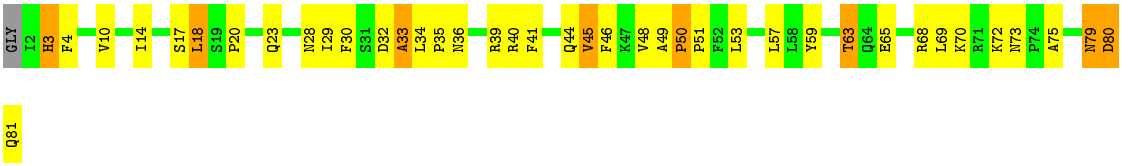
• Molecule 6: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 14 KDA PROTEIN

Chain S:



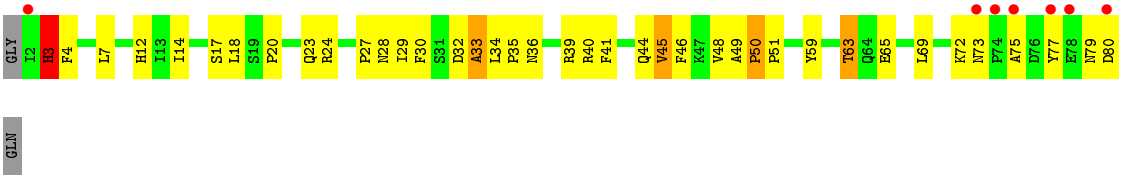
• Molecule 7: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE UBIQUINONE-BINDING PROTEIN QP-C

Chain G:



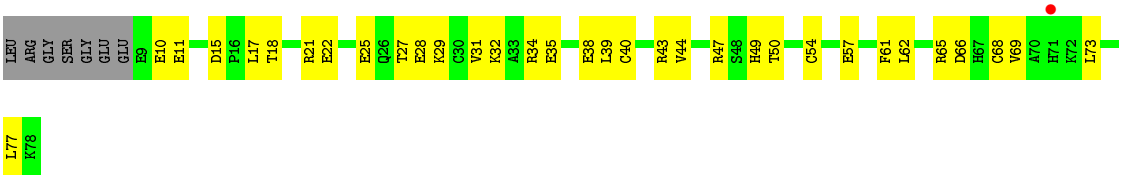
• Molecule 7: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE UBIQUINONE-BINDING PROTEIN QP-C

Chain T:

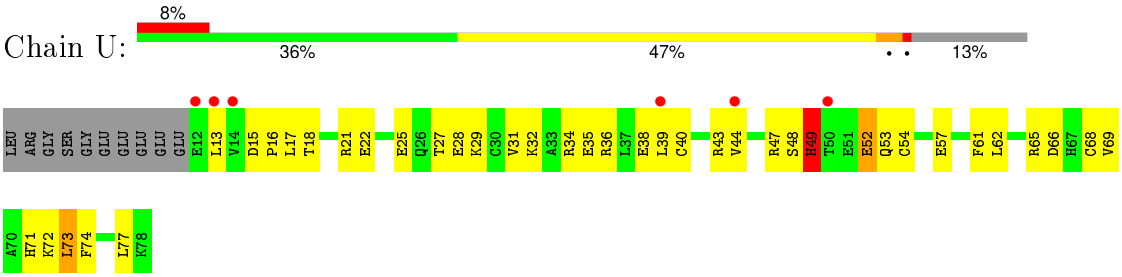


• Molecule 8: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 11 KDA PROTEIN, COMPLEX III SUBUNIT VIII

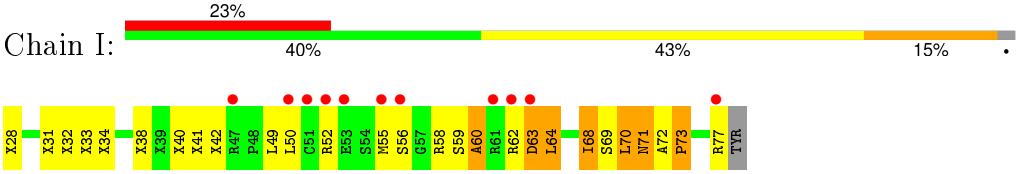
Chain H:



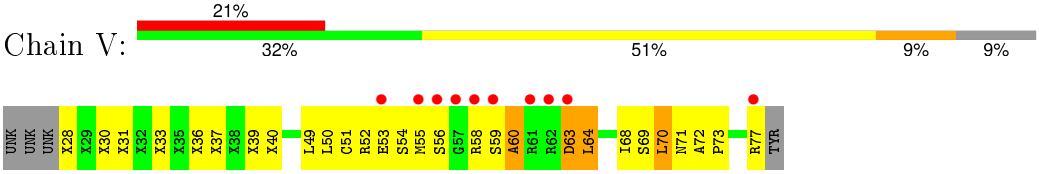
• Molecule 8: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 11 KDA PROTEIN, COMPLEX III SUBUNIT VIII



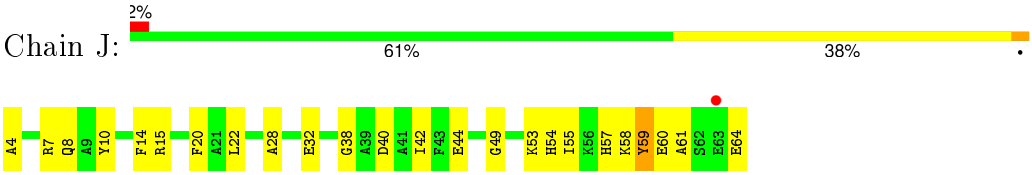
• Molecule 9: CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL



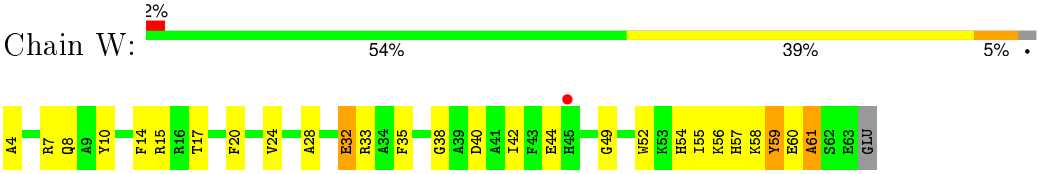
• Molecule 9: CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL



• 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 (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	172.61Å 181.55Å 241.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.93 – 3.06 49.92 – 3.00	Depositor EDS
% Data completeness (in resolution range)	93.8 (28.93-3.06) 93.1 (49.92-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	1.21 (at 3.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.264 , 0.294 0.253 , 0.282	Depositor DCC
R_{free} test set	2644 reflections (2.01%)	DCC
Wilson B-factor (Å^2)	75.1	Xtriage
Anisotropy	0.487	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 61.7	EDS
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.35$	Xtriage
Outliers	0 of 141092 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	32648	wwPDB-VP
Average B, all atoms (Å^2)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.92% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, IKR, CDL, UQ, FES, HEC, 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	0.44	0/3518	0.66	0/4767
1	N	0.45	0/3508	0.66	0/4753
2	B	0.40	0/3191	0.67	0/4326
2	O	0.42	0/3202	0.68	0/4343
3	C	0.51	0/3119	0.68	0/4270
3	P	0.48	0/3114	0.66	0/4263
4	D	0.46	0/1956	0.66	0/2658
4	Q	0.40	0/1956	0.63	0/2658
5	E	0.39	0/1547	0.61	0/2103
5	R	0.40	0/1543	0.62	0/2098
6	F	0.51	0/911	0.70	0/1219
6	S	0.43	0/911	0.64	0/1219
7	G	0.53	0/694	0.70	1/941 (0.1%)
7	T	0.50	0/684	0.71	1/929 (0.1%)
8	H	0.45	0/582	0.66	0/779
8	U	0.37	0/561	0.60	0/751
9	I	0.43	0/218	0.68	0/293
9	V	0.43	0/218	0.67	0/293
10	J	0.45	0/508	0.65	0/682
10	W	0.42	0/490	0.65	0/660
All	All	0.45	0/32431	0.66	2/44005 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
6	F	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	T	18	LEU	CA-CB-CG	5.17	127.19	115.30
7	G	18	LEU	CA-CB-CG	5.11	127.05	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	F	20	TYR	Sidechain

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	3447	0	3362	181	0
1	N	3437	0	3349	204	0
2	B	3137	0	3131	262	0
2	O	3147	0	3146	254	0
3	C	3017	0	3063	148	0
3	P	3012	0	3058	166	0
4	D	1898	0	1846	93	0
4	Q	1898	0	1846	115	0
5	E	1513	0	1478	123	0
5	R	1509	0	1474	126	0
6	F	891	0	893	32	0
6	S	891	0	893	40	0
7	G	672	0	653	48	0
7	T	662	0	645	42	0
8	H	574	0	548	35	0
8	U	553	0	535	42	0
9	I	287	0	251	46	0
9	V	277	0	251	45	0
10	J	497	0	490	20	0
10	W	479	0	478	27	0
11	C	86	0	60	7	0
11	P	86	0	60	5	0
12	C	25	0	20	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	P	25	0	20	3	0
13	C	19	0	17	6	0
13	P	19	0	17	5	0
14	C	40	0	24	1	0
14	D	42	0	28	0	0
14	P	40	0	24	2	0
14	Q	42	0	28	2	0
15	C	70	0	85	1	0
15	E	50	0	77	0	0
15	P	54	0	72	2	0
15	R	50	0	77	1	0
16	C	6	0	8	0	0
16	P	6	0	8	2	0
17	D	43	0	30	2	0
17	Q	43	0	30	2	0
18	D	33	0	39	1	0
18	P	12	0	11	1	0
18	Q	33	0	39	1	0
19	E	4	0	0	2	0
19	R	4	0	0	2	0
20	C	8	0	0	1	0
20	E	1	0	0	0	0
20	P	8	0	0	1	0
20	R	1	0	0	0	0
All	All	32648	0	32164	1865	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 29.

All (1865) 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)
5:E:121:GLN:HG2	5:E:170:ARG:HD3	1.26	1.14
5:E:127:VAL:HG12	5:E:128:LYS:H	1.15	1.09
2:O:76:THR:HG22	2:O:82:SER:H	1.14	1.04
3:P:328:LEU:HD12	7:T:51:PRO:HB3	1.36	1.04
2:B:76:THR:HG22	2:B:82:SER:H	1.17	1.03
2:O:353:THR:HG22	2:O:355:GLU:H	1.24	1.02
2:B:353:THR:HG22	2:B:355:GLU:H	1.24	1.00
2:O:51:ILE:HG12	2:O:204:MET:HG2	1.41	1.00
3:C:328:LEU:HD12	7:G:51:PRO:HB3	1.45	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:178:THR:HG22	1:N:180:ALA:H	1.26	0.97
1:N:102:LEU:HD12	1:N:102:LEU:H	1.31	0.95
4:D:222:MET:HE1	5:E:40:THR:HG23	1.46	0.95
2:B:270:ASN:HD22	2:B:270:ASN:H	1.01	0.94
7:G:41:PHE:O	7:G:45:VAL:HG23	1.68	0.94
9:V:49:LEU:HD13	9:V:55:MET:HG2	1.47	0.94
7:T:80:ASP:HB3	8:U:47:ARG:HH11	1.33	0.93
2:B:51:ILE:HG12	2:B:204:MET:HG2	1.50	0.93
1:A:102:LEU:H	1:A:102:LEU:HD12	1.33	0.93
7:T:41:PHE:O	7:T:45:VAL:HG23	1.69	0.93
4:Q:57:THR:HG22	4:Q:59:ALA:H	1.32	0.92
1:A:178:THR:HG22	1:A:180:ALA:H	1.31	0.92
4:D:57:THR:HG22	4:D:59:ALA:H	1.34	0.91
5:R:45:VAL:HG13	10:W:28:ALA:HA	1.52	0.91
5:E:45:VAL:HG13	10:J:28:ALA:HA	1.52	0.90
1:N:196:VAL:HG11	1:N:383:LEU:HD12	1.53	0.90
2:O:76:THR:CG2	2:O:82:SER:H	1.85	0.90
2:B:76:THR:CG2	2:B:82:SER:H	1.85	0.89
9:I:31:UNK:CA	9:I:73:PRO:HG2	2.03	0.89
4:Q:231:LYS:O	6:S:71:LYS:HE3	1.73	0.89
1:N:170:THR:HG22	1:N:171:THR:H	1.37	0.89
4:D:2:GLU:HB3	7:G:70:LYS:HE2	1.54	0.88
4:Q:47:ALA:H	4:Q:50:ASN:HD22	1.22	0.88
5:R:118:ARG:O	5:R:120:PRO:HD3	1.74	0.87
8:U:43:ARG:HD2	8:U:47:ARG:HH21	1.38	0.87
1:N:60:GLU:OE2	1:N:90:THR:HG22	1.74	0.86
3:P:2:ALA:HB3	3:P:8:SER:HB3	1.56	0.86
3:C:377:MET:HE2	6:F:20:TYR:HB2	1.57	0.86
2:B:168:TYR:HB2	2:B:173:ALA:HB2	1.58	0.86
3:P:23:PRO:HG2	7:T:3:HIS:HB3	1.57	0.85
2:O:37:SER:HB3	2:O:213:HIS:ND1	1.93	0.84
6:F:32:MET:CE	6:F:87:LYS:HG2	2.07	0.84
3:P:301:ILE:HD11	3:P:364:LEU:HD21	1.59	0.84
5:E:83:GLU:HG2	5:E:102:THR:HA	1.59	0.83
2:B:372:VAL:HG13	2:B:378:LEU:HA	1.60	0.83
4:D:231:LYS:O	6:F:71:LYS:HE3	1.78	0.83
6:F:32:MET:HE3	6:F:87:LYS:HG2	1.59	0.83
5:R:134:ILE:HD12	5:R:185:TYR:CD1	2.13	0.83
5:R:171:ILE:HD13	5:R:176:ALA:HB3	1.59	0.83
4:D:47:ALA:H	4:D:50:ASN:HD22	1.22	0.82
5:R:109:GLU:OE1	5:R:123:ASP:HB2	1.79	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:125:MET:CE	12:C:2001:IKR:I1	2.97	0.82
1:A:60:GLU:OE2	1:A:90:THR:HG22	1.79	0.82
1:N:69:LYS:HD2	1:N:70:ARG:HH21	1.44	0.82
1:A:69:LYS:HD2	1:A:70:ARG:HH21	1.45	0.82
1:A:196:VAL:HG11	1:A:383:LEU:HD12	1.62	0.81
3:P:342:GLN:HE21	3:P:343:PRO:HD2	1.46	0.81
3:C:125:MET:HE2	12:C:2001:IKR:I1	2.50	0.81
8:U:32:LYS:O	8:U:36:ARG:HG3	1.79	0.81
7:T:73:ASN:HD21	7:T:75:ALA:HB3	1.46	0.81
2:O:150:VAL:O	2:O:153:GLN:HG3	1.81	0.80
3:P:125:MET:HE2	12:P:3001:IKR:I1	2.51	0.80
3:C:342:GLN:HE21	3:C:343:PRO:HD2	1.46	0.80
5:E:127:VAL:HG12	5:E:128:LYS:N	1.96	0.80
2:B:314:VAL:HG13	9:I:63:ASP:HB3	1.63	0.80
4:Q:222:MET:HE3	5:R:40:THR:HG23	1.64	0.79
2:O:76:THR:HG22	2:O:82:SER:N	1.94	0.79
2:B:150:VAL:O	2:B:153:GLN:HG3	1.81	0.79
2:B:63:LEU:HB2	2:B:182:ARG:HD3	1.65	0.79
5:R:112:VAL:HG21	5:R:170:ARG:NH2	1.97	0.79
4:Q:47:ALA:H	4:Q:50:ASN:ND2	1.80	0.79
4:D:144:ARG:HG2	4:D:147:LEU:HD12	1.63	0.79
5:R:31:ASP:OD2	10:W:7:ARG:HG3	1.83	0.78
2:O:372:VAL:HG13	2:O:378:LEU:HA	1.63	0.78
5:R:117:LEU:HD11	5:R:172:ARG:NH1	1.98	0.78
2:O:168:TYR:HB2	2:O:173:ALA:HB2	1.65	0.78
1:N:105:ASP:O	1:N:109:VAL:HG23	1.84	0.78
2:O:207:VAL:HG12	2:O:208:GLY:H	1.49	0.78
2:O:341:MET:HE2	2:O:341:MET:HA	1.64	0.78
3:P:69:HIS:CD2	3:P:73:ASN:HD22	2.01	0.78
2:O:222:GLN:HG2	2:O:222:GLN:O	1.84	0.78
5:E:76:ILE:HD12	5:E:98:VAL:HG21	1.66	0.78
2:B:306:PRO:HA	9:I:52:ARG:HG3	1.64	0.77
2:O:62:ASN:O	2:O:65:THR:HG22	1.84	0.77
3:C:23:PRO:HG2	7:G:3:HIS:HB3	1.63	0.77
2:B:207:VAL:HG12	2:B:208:GLY:H	1.49	0.77
2:B:57:TYR:HE2	2:B:203:ARG:HH22	1.29	0.77
2:B:76:THR:HG22	2:B:82:SER:N	1.96	0.77
5:E:78:LEU:HD12	5:E:190:ASP:O	1.85	0.77
1:A:112:LEU:O	1:A:116:VAL:HG23	1.84	0.77
9:I:64:LEU:HD12	9:I:77:ARG:C	2.05	0.77
2:O:206:LEU:HD23	2:O:220:ALA:HB2	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:80:ALA:HA	2:B:84:ARG:HH12	1.50	0.77
3:C:120:LEU:HD13	11:C:502:HEM:HAB	1.65	0.76
8:U:43:ARG:HD2	8:U:47:ARG:NH2	1.99	0.76
5:E:164:HIS:HD2	5:E:173:LYS:HB3	1.50	0.76
1:N:182:LEU:O	1:N:186:ILE:HG13	1.86	0.76
1:A:170:THR:HG22	1:A:171:THR:H	1.49	0.76
5:R:78:LEU:HB3	5:R:132:TRP:CZ2	2.20	0.76
3:C:301:ILE:HD11	3:C:364:LEU:HD21	1.67	0.76
1:A:402:VAL:HG22	1:A:406:MET:HE2	1.68	0.76
2:O:157:VAL:HG23	9:V:64:LEU:HD21	1.68	0.76
1:A:50:GLU:HB2	1:A:165:ARG:NH2	2.00	0.76
3:P:125:MET:CE	12:P:3001:IKR:I1	3.04	0.76
2:O:192:HIS:O	2:O:196:GLN:HG3	1.85	0.76
2:O:57:TYR:HE2	2:O:203:ARG:HH22	1.32	0.76
1:A:336:PHE:CZ	3:C:4:ASN:HB3	2.21	0.76
5:R:134:ILE:HD12	5:R:185:TYR:HD1	1.47	0.75
3:P:9:HIS:O	3:P:13:LYS:HB3	1.86	0.75
5:R:83:GLU:HB3	5:R:102:THR:HG22	1.66	0.75
2:O:248:ASN:HD22	2:O:248:ASN:C	1.89	0.75
2:O:283:PRO:HG2	9:V:56:SER:HB2	1.67	0.75
1:N:382:HIS:ND1	1:N:389:ARG:HD2	2.02	0.75
2:B:270:ASN:ND2	2:B:270:ASN:H	1.78	0.75
1:N:170:THR:HG22	1:N:171:THR:N	2.01	0.75
2:O:181:TYR:CE1	2:O:182:ARG:HG3	2.22	0.75
2:B:207:VAL:HG21	2:B:383:GLY:HA2	1.69	0.75
2:B:241:GLY:HA2	2:B:423:SER:HB3	1.69	0.75
3:P:377:MET:HE2	6:S:20:TYR:HB2	1.69	0.75
2:O:241:GLY:HA2	2:O:423:SER:HB3	1.68	0.75
2:O:221:GLU:HG3	2:O:222:GLN:H	1.52	0.74
7:G:81:GLN:HA	8:H:47:ARG:HG2	1.68	0.74
5:R:164:HIS:HD2	5:R:173:LYS:HB3	1.53	0.74
3:P:138:GLN:HB2	3:P:255:GLU:O	1.87	0.74
9:I:70:LEU:HD23	9:I:71:ASN:N	2.02	0.74
2:O:397:VAL:O	2:O:401:LYS:HG2	1.87	0.74
4:Q:221:TYR:HD2	5:R:39:VAL:HG11	1.52	0.74
1:N:35:CYS:HA	1:N:372:THR:HG21	1.69	0.74
2:B:169:LYS:O	2:B:170:THR:HG23	1.87	0.74
6:F:107:TRP:O	6:F:110:LYS:HB3	1.88	0.74
10:W:57:HIS:HA	10:W:60:GLU:HG2	1.69	0.74
3:C:22:LEU:HD21	13:C:2002:UQ:HM32	1.68	0.73
1:A:182:LEU:O	1:A:186:ILE:HG13	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:18:THR:HG23	1:N:24:ARG:HG3	1.70	0.73
2:B:270:ASN:HD22	2:B:270:ASN:N	1.82	0.73
1:A:206:LYS:O	1:A:209:VAL:HG12	1.88	0.73
1:A:443:TRP:CE3	1:A:443:TRP:HA	2.22	0.73
2:O:47:ILE:HD13	2:O:120:MET:CE	2.19	0.73
2:B:62:ASN:O	2:B:65:THR:HG22	1.88	0.73
2:B:168:TYR:CB	2:B:173:ALA:HB2	2.19	0.73
5:E:129:LYS:HG3	5:E:187:PHE:CZ	2.24	0.73
4:D:229:VAL:HG23	7:G:20:PRO:HG3	1.71	0.73
7:G:65:GLU:O	7:G:69:LEU:HG	1.87	0.73
2:O:35:ILE:HD13	2:O:217:LYS:HA	1.69	0.73
7:T:29:ILE:O	7:T:33:ALA:HB3	1.88	0.73
5:E:136:VAL:HG23	5:E:183:PRO:HD3	1.70	0.72
5:E:121:GLN:HG2	5:E:170:ARG:CD	2.14	0.72
5:R:78:LEU:HD13	5:R:132:TRP:NE1	2.03	0.72
1:N:106:MET:HG3	1:N:203:ILE:HD13	1.71	0.72
3:P:27:ASN:ND2	3:P:209:PRO:HG2	2.04	0.72
4:D:232:SER:HB3	7:G:23:GLN:HE22	1.54	0.72
3:C:9:HIS:O	3:C:13:LYS:HB3	1.89	0.72
3:C:50:LEU:O	3:C:54:MET:HG3	1.90	0.72
1:N:321:GLY:HA2	1:N:342:TRP:HZ2	1.55	0.72
2:B:56:ARG:NH1	2:B:172:LEU:HG	2.05	0.72
1:N:206:LYS:O	1:N:209:VAL:HG12	1.89	0.72
1:N:112:LEU:O	1:N:116:VAL:HG23	1.89	0.72
1:N:336:PHE:CZ	3:P:4:ASN:HB3	2.25	0.72
1:N:85:HIS:CD2	2:O:284:LEU:HD22	2.25	0.71
2:B:56:ARG:HH12	2:B:172:LEU:HG	1.55	0.71
3:C:125:MET:HE1	12:C:2001:IKR:I1	2.60	0.71
4:Q:144:ARG:HG2	4:Q:147:LEU:HD12	1.72	0.71
2:B:306:PRO:HA	9:I:52:ARG:CG	2.19	0.71
2:B:57:TYR:CE2	2:B:203:ARG:NH2	2.58	0.71
7:G:80:ASP:HB3	8:H:50:THR:HA	1.72	0.71
5:E:106:ILE:O	5:E:110:ALA:HB3	1.90	0.71
5:E:31:ASP:OD2	10:J:7:ARG:HG3	1.90	0.71
14:P:3004:CDL:OA4	7:T:40:ARG:HD2	1.89	0.71
1:A:7:THR:HG21	2:B:113:ARG:HD2	1.71	0.71
2:B:341:MET:HE2	2:B:341:MET:HA	1.71	0.71
7:G:29:ILE:O	7:G:33:ALA:HB3	1.91	0.71
15:C:2007:PEE:H7	7:G:44:GLN:HE21	1.54	0.71
2:O:56:ARG:HH12	2:O:172:LEU:HG	1.56	0.71
6:S:13:MET:HA	6:S:16:ILE:HB	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:231:LEU:HD23	1:N:232:PRO:HD2	1.73	0.71
2:B:47:ILE:HD13	2:B:120:MET:CE	2.21	0.71
2:O:56:ARG:NH1	2:O:172:LEU:HG	2.05	0.71
2:B:166:ALA:HB2	2:B:244:ILE:HG13	1.73	0.71
2:B:37:SER:HB3	2:B:213:HIS:ND1	2.06	0.71
6:F:32:MET:HE3	6:F:87:LYS:CG	2.21	0.70
5:R:120:PRO:O	5:R:121:GLN:HG3	1.90	0.70
3:P:101:ARG:C	3:P:101:ARG:HD2	2.12	0.70
2:O:422:LYS:O	2:O:436:LEU:HD21	1.91	0.70
4:Q:221:TYR:CD2	5:R:39:VAL:HG11	2.26	0.70
7:G:73:ASN:HD21	7:G:75:ALA:HB3	1.57	0.70
5:R:112:VAL:HG21	5:R:170:ARG:HH22	1.54	0.70
2:O:47:ILE:HD11	2:O:116:VAL:HG13	1.73	0.70
2:O:338:ARG:HH11	2:O:338:ARG:HG3	1.54	0.70
3:P:245:LEU:O	4:Q:201:ARG:HD3	1.91	0.70
4:Q:74:PRO:HB2	4:Q:78:GLY:HA2	1.73	0.70
7:T:50:PRO:HB2	7:T:51:PRO:CD	2.22	0.70
1:A:321:GLY:HA2	1:A:342:TRP:HZ2	1.57	0.70
4:D:74:PRO:HB2	4:D:78:GLY:HA2	1.72	0.70
1:N:305:HIS:HB3	9:V:36:UNK:CB	2.21	0.70
5:R:77:LYS:HA	5:R:191:ASP:O	1.92	0.70
3:P:238:THR:HB	3:P:239:PRO:HD3	1.74	0.69
1:N:443:TRP:CE3	1:N:443:TRP:HA	2.25	0.69
1:A:178:THR:HB	1:A:181:ASP:OD1	1.92	0.69
2:O:57:TYR:CE2	2:O:203:ARG:NH2	2.59	0.69
2:B:35:ILE:HD13	2:B:217:LYS:HA	1.73	0.69
2:B:248:ASN:HD22	2:B:248:ASN:C	1.94	0.69
7:T:73:ASN:ND2	7:T:75:ALA:HB3	2.07	0.69
2:O:63:LEU:HB2	2:O:182:ARG:HD3	1.73	0.69
2:B:397:VAL:O	2:B:401:LYS:HG2	1.91	0.69
4:D:47:ALA:H	4:D:50:ASN:ND2	1.90	0.69
5:E:129:LYS:HB3	5:E:132:TRP:HB2	1.75	0.69
2:B:47:ILE:HD11	2:B:116:VAL:HG13	1.75	0.69
1:N:50:GLU:HB2	1:N:165:ARG:NH2	2.08	0.69
2:O:286:LYS:HE2	2:O:287:ARG:NH1	2.08	0.69
4:Q:8:PRO:HG2	4:Q:10:PHE:CE1	2.27	0.69
2:O:238:THR:HG22	2:O:239:TYR:N	2.09	0.68
5:E:86:ASN:HD22	5:E:148:ALA:HB2	1.56	0.68
1:N:344:ARG:HG3	1:N:344:ARG:HH11	1.58	0.68
17:Q:501:HEC:HMB1	17:Q:501:HEC:HBB3	1.75	0.68
2:B:154:SER:O	2:B:157:VAL:HG12	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:248:ASN:ND2	2:O:250:HIS:H	1.92	0.68
1:N:196:VAL:CG1	1:N:383:LEU:HD12	2.22	0.68
5:E:81:ILE:HB	5:E:132:TRP:HH2	1.58	0.68
2:O:154:SER:O	2:O:157:VAL:HG12	1.94	0.68
2:O:96:LEU:HB3	9:V:70:LEU:HD22	1.76	0.68
7:G:36:ASN:OD1	7:G:39:ARG:NH1	2.27	0.68
1:A:85:HIS:CD2	2:B:284:LEU:HD22	2.28	0.68
2:B:238:THR:HG22	2:B:239:TYR:H	1.59	0.68
1:A:170:THR:HG22	1:A:171:THR:N	2.08	0.68
7:G:50:PRO:HB2	7:G:51:PRO:CD	2.24	0.67
1:A:443:TRP:HE3	1:A:443:TRP:HA	1.59	0.67
2:O:27:THR:HG22	2:O:28:LYS:N	2.09	0.67
6:S:95:LYS:O	6:S:99:ARG:HG3	1.95	0.67
1:A:50:GLU:HB2	1:A:165:ARG:HH21	1.56	0.67
3:C:328:LEU:CD1	7:G:51:PRO:HB3	2.23	0.67
4:Q:181:GLN:HA	8:U:77:LEU:HD22	1.76	0.67
15:P:3007:PEE:H7	7:T:44:GLN:HE21	1.59	0.67
1:N:402:VAL:HG22	1:N:406:MET:HE2	1.76	0.67
2:O:168:TYR:CB	2:O:173:ALA:HB2	2.23	0.67
3:C:138:GLN:HB2	3:C:255:GLU:O	1.95	0.67
1:A:109:VAL:HA	1:A:112:LEU:HD12	1.76	0.67
9:V:64:LEU:HD12	9:V:77:ARG:C	2.15	0.67
4:Q:95:TYR:CD2	4:Q:101:ALA:HA	2.29	0.67
5:E:129:LYS:HG3	5:E:187:PHE:CE2	2.30	0.67
1:A:106:MET:HG3	1:A:203:ILE:HD13	1.77	0.67
5:R:117:LEU:HD11	5:R:172:ARG:HH11	1.58	0.67
5:R:177:PRO:HG2	5:R:178:TYR:H	1.59	0.66
3:P:50:LEU:O	3:P:54:MET:HG3	1.96	0.66
10:J:38:GLY:O	10:J:42:ILE:HG13	1.95	0.66
2:O:361:LYS:O	2:O:365:LYS:HG3	1.94	0.66
10:W:49:GLY:N	10:W:54:HIS:ND1	2.44	0.66
2:B:374:THR:HG22	2:B:376:GLN:H	1.61	0.66
8:U:27:THR:O	8:U:31:VAL:HG23	1.96	0.66
3:C:101:ARG:C	3:C:101:ARG:HD2	2.15	0.66
4:D:57:THR:HG22	4:D:59:ALA:N	2.10	0.66
5:R:113:ASP:HB2	5:R:116:LYS:HB2	1.78	0.66
4:Q:102:ARG:HB3	4:Q:107:GLY:HA2	1.77	0.66
7:T:65:GLU:O	7:T:69:LEU:HG	1.95	0.66
2:O:169:LYS:O	2:O:170:THR:HG23	1.96	0.66
5:E:78:LEU:HD11	5:E:187:PHE:CE2	2.31	0.66
3:C:69:HIS:CD2	3:C:73:ASN:HD22	2.13	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:238:THR:HB	3:C:239:PRO:HD3	1.78	0.66
2:O:31:ASN:N	2:O:31:ASN:HD22	1.93	0.66
2:B:283:PRO:HG2	9:I:56:SER:HB2	1.77	0.65
2:O:314:VAL:HG13	9:V:63:ASP:HB3	1.76	0.65
2:O:325:TYR:HD1	9:V:60:ALA:CB	2.09	0.65
3:P:18:SER:HB2	3:P:202:HIS:HE1	1.61	0.65
4:D:181:GLN:HA	8:H:77:LEU:HD22	1.79	0.65
5:E:165:TYR:HA	5:E:170:ARG:O	1.96	0.65
9:I:49:LEU:HD13	9:I:55:MET:HG2	1.78	0.65
2:O:238:THR:HG22	2:O:239:TYR:H	1.60	0.65
2:O:109:VAL:HG21	2:O:119:VAL:HG12	1.77	0.65
4:Q:57:THR:HG22	4:Q:59:ALA:N	2.10	0.65
10:J:49:GLY:N	10:J:54:HIS:ND1	2.45	0.65
2:O:166:ALA:HB1	2:O:242:GLY:O	1.97	0.65
1:N:321:GLY:HA2	1:N:342:TRP:CZ2	2.32	0.65
1:A:35:CYS:HA	1:A:372:THR:HG21	1.77	0.65
1:N:371:GLY:O	1:N:375:VAL:HG23	1.95	0.65
2:O:166:ALA:HB2	2:O:244:ILE:HG13	1.79	0.65
3:P:173:ASN:N	3:P:174:PRO:HD2	2.12	0.65
5:E:116:LYS:H	5:E:116:LYS:HD2	1.62	0.65
2:B:264:VAL:HG23	2:B:316:TYR:C	2.18	0.64
1:A:382:HIS:ND1	1:A:389:ARG:HD2	2.11	0.64
2:O:257:VAL:HG22	2:O:424:MET:HG3	1.77	0.64
2:B:338:ARG:HG3	2:B:338:ARG:HH11	1.61	0.64
3:C:105:TYR:CD2	3:C:209:PRO:HA	2.33	0.64
4:Q:237:TYR:HB2	6:S:60:PHE:CG	2.31	0.64
1:N:7:THR:HG21	2:O:113:ARG:HD2	1.80	0.64
2:B:238:THR:HG22	2:B:239:TYR:N	2.11	0.64
9:I:71:ASN:HD22	9:I:71:ASN:H	1.44	0.64
3:C:173:ASN:N	3:C:174:PRO:HD2	2.12	0.64
2:B:325:TYR:HD1	9:I:60:ALA:HB3	1.61	0.64
3:C:25:PRO:HB2	3:C:28:ILE:HG23	1.79	0.64
10:W:38:GLY:O	10:W:42:ILE:HG13	1.97	0.64
2:B:361:LYS:O	2:B:365:LYS:HG3	1.97	0.64
2:B:192:HIS:O	2:B:196:GLN:HG3	1.98	0.64
1:A:117:VAL:HG23	1:A:118:GLN:N	2.12	0.64
5:E:166:ASP:OD2	5:E:170:ARG:HB2	1.97	0.64
2:B:181:TYR:CE1	2:B:182:ARG:HG3	2.32	0.64
5:E:69:LEU:O	5:E:72:SER:HB3	1.97	0.64
3:P:25:PRO:HB2	3:P:28:ILE:HG23	1.79	0.64
3:P:328:LEU:CD1	7:T:51:PRO:HB3	2.21	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:178:THR:HB	1:N:181:ASP:OD1	1.98	0.64
2:O:169:LYS:HG3	2:O:240:TRP:HB2	1.79	0.64
5:E:190:ASP:C	5:E:192:LEU:H	2.00	0.64
2:O:47:ILE:CD1	2:O:116:VAL:HG13	2.28	0.64
2:B:75:LEU:HD22	2:B:136:GLU:HB3	1.80	0.64
4:D:102:ARG:NH1	4:D:107:GLY:O	2.31	0.64
17:D:501:HEC:HBB3	17:D:501:HEC:HMB1	1.78	0.64
2:O:248:ASN:HD21	2:O:250:HIS:HB2	1.63	0.63
2:O:325:TYR:HD2	2:O:326:THR:N	1.96	0.63
1:N:49:ASN:ND2	1:N:51:LYS:H	1.95	0.63
3:C:328:LEU:HD12	7:G:51:PRO:CB	2.26	0.63
2:O:80:ALA:HA	2:O:84:ARG:HH12	1.63	0.63
2:O:56:ARG:HA	2:O:171:ALA:O	1.97	0.63
2:O:96:LEU:HD13	2:O:109:VAL:HG12	1.81	0.63
1:N:332:ASP:HB2	1:N:430:GLN:HG2	1.81	0.63
5:R:45:VAL:HG13	10:W:28:ALA:CA	2.27	0.63
5:E:106:ILE:C	5:E:110:ALA:HB3	2.19	0.63
2:B:295:LEU:O	2:B:299:VAL:HG23	1.98	0.63
7:T:36:ASN:OD1	7:T:39:ARG:NH1	2.32	0.63
2:B:47:ILE:CD1	2:B:116:VAL:HG13	2.28	0.63
4:Q:54:VAL:HG11	4:Q:192:TRP:NE1	2.13	0.63
4:Q:229:VAL:HG23	7:T:20:PRO:HG3	1.80	0.63
5:E:96:LEU:HD12	5:E:135:LEU:O	1.99	0.63
1:N:443:TRP:HE3	1:N:443:TRP:HA	1.61	0.63
1:N:242:ARG:HH12	1:N:432:LEU:HA	1.64	0.63
2:O:56:ARG:HG3	2:O:56:ARG:HH11	1.64	0.63
3:C:18:SER:HB2	3:C:202:HIS:HE1	1.64	0.63
1:A:186:ILE:HG23	1:A:190:PHE:CD1	2.34	0.63
2:B:422:LYS:O	2:B:436:LEU:HD21	1.97	0.63
1:A:321:GLY:HA2	1:A:342:TRP:CZ2	2.33	0.63
1:A:249:PRO:HG2	1:A:250:VAL:H	1.64	0.63
2:O:359:LYS:O	2:O:363:GLN:HG3	1.99	0.63
2:B:57:TYR:CD1	2:B:57:TYR:N	2.67	0.63
1:N:161:THR:HG21	1:N:235:ARG:H	1.62	0.63
3:C:198:LEU:HD13	13:C:2002:UQ:HM53	1.81	0.62
4:D:221:TYR:CD2	5:E:39:VAL:HG11	2.34	0.62
2:O:399:ALA:O	2:O:402:ILE:HG22	1.99	0.62
9:I:32:UNK:N	9:I:73:PRO:HG2	2.14	0.62
1:N:336:PHE:CE2	3:P:4:ASN:HB3	2.34	0.62
4:Q:26:VAL:HG22	4:Q:188:THR:HG22	1.81	0.62
2:B:166:ALA:HB1	2:B:242:GLY:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:V:70:LEU:HD23	9:V:71:ASN:N	2.13	0.62
4:D:26:VAL:HG22	4:D:188:THR:HG22	1.81	0.62
2:O:417:PHE:O	2:O:422:LYS:HE3	1.99	0.62
4:D:102:ARG:HB3	4:D:107:GLY:HA2	1.81	0.62
1:N:249:PRO:HG2	1:N:250:VAL:H	1.62	0.62
2:B:56:ARG:HG3	2:B:56:ARG:HH11	1.64	0.62
8:H:40:CYS:O	8:H:44:VAL:HG23	2.00	0.62
3:P:105:TYR:CD2	3:P:209:PRO:HA	2.35	0.62
3:P:67:VAL:HG12	16:P:3011:GOL:H31	1.82	0.62
5:R:96:LEU:HD12	5:R:135:LEU:O	2.00	0.62
1:A:231:LEU:HD23	1:A:232:PRO:HD2	1.81	0.62
3:P:328:LEU:HD12	7:T:51:PRO:CB	2.22	0.61
2:O:424:MET:HG2	2:O:425:ALA:N	2.15	0.61
2:B:417:PHE:O	2:B:422:LYS:HE3	1.99	0.61
1:N:109:VAL:HA	1:N:112:LEU:HD12	1.82	0.61
4:Q:70:VAL:HG21	4:Q:83:ARG:CZ	2.30	0.61
2:B:21:ALA:O	2:B:22:GLU:HB2	1.99	0.61
5:R:165:TYR:HA	5:R:170:ARG:O	2.00	0.61
5:R:81:ILE:HG22	5:R:100:HIS:HB2	1.82	0.61
1:A:111:GLU:HG3	1:A:215:HIS:CD2	2.35	0.61
3:P:20:ILE:HG22	3:P:21:ASP:OD1	2.00	0.61
2:O:219:VAL:O	2:O:223:PHE:HB2	1.99	0.61
1:N:111:GLU:HG3	1:N:215:HIS:CD2	2.34	0.61
2:B:157:VAL:HG23	9:I:64:LEU:HD21	1.83	0.61
2:O:286:LYS:HE2	2:O:287:ARG:HH12	1.65	0.61
5:R:129:LYS:HB3	5:R:131:GLU:OE1	1.99	0.61
1:N:85:HIS:NE2	2:O:284:LEU:HD22	2.15	0.61
3:P:70:THR:HA	3:P:74:VAL:HG23	1.82	0.61
1:A:191:LYS:O	1:A:195:MET:HG3	1.99	0.61
9:I:72:ALA:HB1	9:I:73:PRO:CD	2.30	0.61
8:H:44:VAL:HG21	8:H:54:CYS:SG	2.40	0.61
14:C:2004:CDL:OA4	7:G:40:ARG:HD2	2.01	0.61
3:P:49:GLY:C	11:P:501:HEM:HAC	2.21	0.61
3:C:347:PRO:O	3:C:350:ILE:HG22	2.01	0.61
2:O:374:THR:HG22	2:O:376:GLN:H	1.65	0.61
2:O:338:ARG:NH1	2:O:338:ARG:HG3	2.16	0.61
2:B:248:ASN:HD21	2:B:250:HIS:HB2	1.66	0.61
2:B:341:MET:HE3	2:B:417:PHE:CE2	2.36	0.61
5:R:69:LEU:O	5:R:72:SER:HB3	2.00	0.61
3:P:199:THR:HA	18:P:2010:BOG:O1	2.01	0.61
2:O:325:TYR:HD1	9:V:60:ALA:HB3	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:75:LEU:HD22	2:O:136:GLU:HB3	1.83	0.61
3:C:127:THR:HG21	11:C:501:HEM:HBB2	1.82	0.61
1:N:138:LEU:HD21	1:N:168:GLU:HB3	1.83	0.61
7:T:77:TYR:C	7:T:79:ASN:H	2.04	0.61
1:A:178:THR:HG22	1:A:179:ARG:N	2.14	0.60
3:C:27:ASN:ND2	3:C:209:PRO:HG2	2.16	0.60
2:B:277:HIS:CD2	2:B:364:LEU:HD13	2.36	0.60
1:N:395:TRP:HA	1:N:395:TRP:CE3	2.36	0.60
2:O:207:VAL:HG21	2:O:383:GLY:HA2	1.82	0.60
3:P:9:HIS:HD2	3:P:12:LEU:H	1.49	0.60
2:B:33:LEU:HD21	2:B:224:LEU:HD12	1.83	0.60
5:R:148:ALA:HB2	5:R:156:TYR:CD2	2.36	0.60
6:S:67:ASP:CG	6:S:71:LYS:HZ3	2.04	0.60
1:N:186:ILE:HG23	1:N:190:PHE:CD1	2.37	0.60
2:B:341:MET:HE3	2:B:417:PHE:HE2	1.65	0.60
2:B:394:ALA:HB3	2:B:397:VAL:HG23	1.84	0.60
1:N:327:ASP:HB3	1:N:328:PRO:HD2	1.84	0.60
2:B:292:THR:O	2:B:292:THR:HG22	2.02	0.60
5:E:81:ILE:HB	5:E:132:TRP:CH2	2.36	0.60
2:B:399:ALA:O	2:B:402:ILE:HG22	2.01	0.60
2:B:325:TYR:HD2	2:B:326:THR:N	1.99	0.60
2:B:132:PHE:CD1	2:B:191:LEU:HB3	2.37	0.60
2:O:295:LEU:O	2:O:299:VAL:HG23	2.02	0.60
5:E:78:LEU:HD11	5:E:187:PHE:CD2	2.37	0.60
1:A:406:MET:O	1:A:410:VAL:HG23	2.01	0.60
2:B:96:LEU:HD13	2:B:109:VAL:HG12	1.82	0.60
1:A:85:HIS:NE2	2:B:284:LEU:HD22	2.16	0.60
2:O:219:VAL:HG13	2:O:223:PHE:HD1	1.67	0.60
2:B:201:SER:OG	2:B:228:SER:HA	2.00	0.60
5:E:45:VAL:HG13	10:J:28:ALA:CA	2.28	0.59
8:H:18:THR:O	8:H:22:GLU:HG3	2.02	0.59
5:E:86:ASN:OD1	5:E:99:ARG:HB2	2.02	0.59
7:T:24:ARG:HB2	7:T:27:PRO:HB3	1.84	0.59
2:B:31:ASN:N	2:B:31:ASN:HD22	2.00	0.59
2:O:341:MET:HE3	2:O:417:PHE:CE2	2.37	0.59
4:D:95:TYR:CD2	4:D:101:ALA:HA	2.36	0.59
9:V:30:UNK:HG3	9:V:31:UNK:N	2.17	0.59
5:R:49:TYR:HE1	10:W:32:GLU:HG3	1.67	0.59
6:S:32:MET:HE3	6:S:87:LYS:HB2	1.83	0.59
1:N:178:THR:HG22	1:N:179:ARG:N	2.17	0.59
1:N:35:CYS:SG	1:N:203:ILE:HD11	2.41	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:62:LEU:O	8:U:66:ASP:HB2	2.02	0.59
4:D:70:VAL:HG21	4:D:83:ARG:CZ	2.33	0.59
8:H:27:THR:HG22	8:H:29:LYS:H	1.68	0.59
1:A:156:THR:HA	5:E:7:VAL:HG21	1.84	0.59
1:A:371:GLY:O	1:A:375:VAL:HG23	2.02	0.59
2:B:168:TYR:CE2	2:B:172:LEU:HD12	2.37	0.59
2:O:341:MET:CE	2:O:417:PHE:HE2	2.15	0.59
2:O:402:ILE:HD13	2:O:402:ILE:C	2.23	0.59
1:A:332:ASP:HB2	1:A:430:GLN:HG2	1.83	0.59
3:P:22:LEU:HD21	13:P:3002:UQ:HM32	1.84	0.59
2:B:248:ASN:ND2	2:B:250:HIS:H	2.01	0.59
4:D:195:GLU:OE1	4:D:201:ARG:NH2	2.36	0.59
2:B:286:LYS:HE2	2:B:287:ARG:NH1	2.17	0.59
2:B:424:MET:HG2	2:B:425:ALA:N	2.17	0.59
1:N:145:MET:HB3	1:N:252:HIS:CD2	2.37	0.59
7:T:72:LYS:CE	8:U:57:GLU:OE1	2.50	0.59
3:C:278:ALA:HB1	3:C:295:LEU:CD1	2.33	0.59
5:R:166:ASP:OD2	5:R:170:ARG:HB2	2.03	0.59
5:R:187:PHE:O	5:R:188:VAL:HG13	2.03	0.59
3:C:9:HIS:HD2	3:C:12:LEU:H	1.50	0.59
2:B:341:MET:CE	2:B:417:PHE:HE2	2.16	0.59
1:N:317:THR:HG23	1:N:318:GLY:N	2.18	0.59
2:O:248:ASN:HD22	2:O:249:GLY:N	2.00	0.59
1:A:242:ARG:HH12	1:A:432:LEU:HA	1.67	0.59
10:W:14:PHE:CD2	10:W:14:PHE:N	2.69	0.59
5:E:165:TYR:CD2	5:E:180:LEU:HG	2.38	0.58
2:O:239:TYR:HE2	2:O:241:GLY:CA	2.16	0.58
2:B:97:SER:HB3	9:I:69:SER:HA	1.85	0.58
13:P:3002:UQ:HM51	13:P:3002:UQ:C8	2.33	0.58
2:B:327:ILE:HD11	9:I:58:ARG:O	2.04	0.58
2:O:71:LEU:O	2:O:74:PRO:HD2	2.02	0.58
1:A:64:PHE:HA	1:A:75:PHE:HE2	1.68	0.58
5:R:86:ASN:OD1	5:R:99:ARG:HB2	2.03	0.58
5:R:82:PRO:O	5:R:100:HIS:HB3	2.03	0.58
13:C:2002:UQ:HM51	13:C:2002:UQ:C8	2.33	0.58
3:P:31:TRP:O	3:P:101:ARG:HG3	2.03	0.58
7:G:73:ASN:ND2	7:G:75:ALA:HB3	2.18	0.58
3:C:151:PHE:HB2	3:C:162:VAL:HG22	1.84	0.58
8:U:28:GLU:O	8:U:32:LYS:HG3	2.04	0.58
1:N:406:MET:O	1:N:410:VAL:HG23	2.03	0.58
3:C:245:LEU:O	4:D:201:ARG:HD3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:439:SER:HA	1:N:442:TYR:CE2	2.38	0.58
1:A:196:VAL:CG1	1:A:383:LEU:HD12	2.32	0.58
2:O:207:VAL:HG12	2:O:208:GLY:N	2.18	0.58
5:E:76:ILE:CD1	5:E:98:VAL:HG21	2.33	0.58
8:H:27:THR:O	8:H:31:VAL:HG23	2.02	0.58
2:B:258:VAL:HG21	2:B:321:LEU:HD22	1.86	0.58
1:A:362:ARG:O	1:A:365:MET:HG2	2.03	0.58
2:B:207:VAL:HG12	2:B:208:GLY:N	2.18	0.58
2:B:62:ASN:ND2	2:B:65:THR:HG21	2.18	0.58
2:B:29:LEU:HB3	2:B:30:PRO:HD2	1.85	0.58
2:B:262:ALA:O	2:B:320:GLY:HA3	2.03	0.58
4:Q:24:SER:OG	10:W:55:ILE:HG21	2.04	0.58
5:E:102:THR:HB	5:E:103:GLN:OE1	2.03	0.58
3:P:142:TRP:O	3:P:146:VAL:HG23	2.03	0.58
5:R:49:TYR:CE1	10:W:32:GLU:HG3	2.39	0.58
1:N:38:GLY:HA3	1:N:98:TYR:HA	1.86	0.58
10:W:56:LYS:HG2	10:W:60:GLU:OE1	2.03	0.58
2:O:292:THR:HG22	2:O:292:THR:O	2.02	0.58
3:P:106:GLY:HA2	3:P:108:TYR:CE2	2.38	0.58
8:U:40:CYS:O	8:U:44:VAL:HG23	2.03	0.57
4:Q:218:LEU:HD11	5:R:42:THR:HG22	1.85	0.57
3:P:127:THR:HG21	11:P:501:HEM:HBB2	1.85	0.57
2:B:124:LEU:HD11	2:B:223:PHE:HB3	1.85	0.57
2:O:357:VAL:HG12	2:O:361:LYS:HE3	1.85	0.57
4:D:221:TYR:HD2	5:E:39:VAL:HG11	1.69	0.57
9:I:31:UNK:C	9:I:73:PRO:HG2	2.33	0.57
3:P:27:ASN:HD22	3:P:209:PRO:HG2	1.70	0.57
1:N:342:TRP:O	1:N:345:LEU:HB2	2.03	0.57
2:B:26:ILE:O	2:B:26:ILE:HG12	2.03	0.57
8:H:34:ARG:HD2	8:H:38:GLU:OE2	2.05	0.57
3:P:145:THR:O	3:P:149:ASN:HB2	2.04	0.57
2:O:291:VAL:HA	2:O:297:GLN:HE21	1.67	0.57
9:I:33:UNK:CG	9:I:73:PRO:HB3	2.35	0.57
2:B:259:THR:HG22	2:B:260:GLU:N	2.19	0.57
5:E:29:SER:HA	5:E:32:ARG:NH2	2.19	0.57
2:B:407:SER:O	2:B:411:VAL:HG23	2.04	0.57
3:P:40:VAL:HA	3:P:43:MET:HE3	1.87	0.57
1:N:117:VAL:HG23	1:N:118:GLN:N	2.20	0.57
2:B:109:VAL:HG21	2:B:119:VAL:HG12	1.87	0.57
5:E:136:VAL:O	5:E:138:VAL:N	2.36	0.57
1:A:105:ASP:O	1:A:109:VAL:HG23	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:171:ILE:CD1	5:R:176:ALA:HB3	2.33	0.57
2:O:57:TYR:N	2:O:57:TYR:CD1	2.73	0.57
1:N:50:GLU:HB2	1:N:165:ARG:HH21	1.67	0.57
2:O:97:SER:HB3	9:V:69:SER:HA	1.85	0.57
1:A:85:HIS:HB2	1:A:100:LYS:HB2	1.87	0.57
8:H:10:GLU:O	8:H:11:GLU:HG3	2.04	0.57
2:O:277:HIS:CD2	2:O:364:LEU:HD13	2.40	0.57
8:U:40:CYS:HA	8:U:43:ARG:NH1	2.19	0.57
6:S:99:ARG:NH1	6:S:99:ARG:HB3	2.20	0.57
5:R:29:SER:HA	5:R:32:ARG:NH2	2.19	0.57
3:P:219:ILE:HB	3:P:224:TYR:CD1	2.40	0.57
3:P:37:LEU:HD21	3:P:233:LEU:HA	1.86	0.57
2:B:46:ARG:HG3	2:B:379:LEU:HD22	1.87	0.57
4:D:8:PRO:HG2	4:D:10:PHE:CE1	2.40	0.57
1:A:197:LEU:HD22	1:A:216:PHE:HE1	1.69	0.57
7:T:80:ASP:HB3	8:U:47:ARG:NH1	2.14	0.57
5:R:153:PHE:HE2	5:R:172:ARG:HH21	1.53	0.57
5:R:118:ARG:NH2	5:R:174:GLY:O	2.38	0.56
2:B:63:LEU:HB2	2:B:182:ARG:CD	2.34	0.56
2:O:259:THR:HG22	2:O:260:GLU:N	2.20	0.56
2:B:76:THR:HG22	2:B:81:SER:HA	1.87	0.56
5:R:78:LEU:HB3	5:R:132:TRP:HZ2	1.65	0.56
3:P:236:MET:O	3:P:239:PRO:HD2	2.05	0.56
2:B:71:LEU:O	2:B:74:PRO:HD2	2.05	0.56
8:H:62:LEU:O	8:H:66:ASP:HB2	2.05	0.56
3:P:347:PRO:O	3:P:350:ILE:HG22	2.04	0.56
2:B:169:LYS:HG3	2:B:240:TRP:HB2	1.86	0.56
1:A:402:VAL:HG22	1:A:406:MET:CE	2.34	0.56
2:B:239:TYR:HE2	2:B:241:GLY:CA	2.18	0.56
7:G:81:GLN:HA	8:H:47:ARG:CG	2.34	0.56
1:A:41:ILE:HD13	1:A:190:PHE:CD2	2.40	0.56
2:B:357:VAL:HG12	2:B:361:LYS:HE3	1.87	0.56
3:C:70:THR:HA	3:C:74:VAL:HG23	1.87	0.56
2:B:337:ILE:HD12	2:B:434:PRO:HD2	1.88	0.56
2:B:348:ALA:HA	2:B:414:ALA:HB3	1.88	0.56
8:U:18:THR:O	8:U:22:GLU:HG3	2.04	0.56
3:C:329:LEU:O	3:C:332:ASN:HB3	2.05	0.56
3:P:329:LEU:O	3:P:332:ASN:HB3	2.04	0.56
1:A:58:PHE:HB3	1:A:182:LEU:HD21	1.87	0.56
5:E:86:ASN:HB2	5:E:99:ARG:HE	1.71	0.56
2:O:348:ALA:HA	2:O:414:ALA:HB3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:247:SER:OG	3:C:250:LEU:HB2	2.06	0.56
1:A:395:TRP:HA	1:A:395:TRP:CE3	2.40	0.56
2:B:132:PHE:CE1	2:B:191:LEU:HB3	2.40	0.56
5:R:136:VAL:O	5:R:138:VAL:N	2.38	0.56
1:A:137:GLU:O	1:A:141:MET:HG3	2.05	0.56
10:W:60:GLU:O	10:W:61:ALA:HB2	2.06	0.56
2:B:130:PRO:HB2	2:B:132:PHE:CE2	2.41	0.56
1:N:307:PHE:CD1	1:N:307:PHE:C	2.78	0.56
5:E:187:PHE:C	5:E:189:GLY:H	2.07	0.56
3:C:350:ILE:HG23	3:C:351:ILE:N	2.21	0.56
10:W:40:ASP:O	10:W:44:GLU:HG3	2.05	0.56
1:N:390:ILE:HG23	1:N:394:GLU:OE1	2.05	0.56
5:E:178:TYR:HD1	5:E:178:TYR:H	1.54	0.56
1:N:41:ILE:HD13	1:N:190:PHE:CD2	2.40	0.56
1:N:402:VAL:HG22	1:N:406:MET:CE	2.36	0.56
2:O:357:VAL:O	2:O:361:LYS:HG3	2.06	0.56
9:V:59:SER:O	9:V:60:ALA:C	2.43	0.56
2:O:414:ALA:O	2:O:418:VAL:HG23	2.06	0.56
4:D:54:VAL:HG11	4:D:192:TRP:NE1	2.20	0.56
1:N:137:GLU:O	1:N:141:MET:HG3	2.06	0.56
3:C:222:HIS:HA	3:C:226:SER:OG	2.06	0.56
2:O:337:ILE:HD12	2:O:434:PRO:HD2	1.88	0.56
1:N:64:PHE:HA	1:N:75:PHE:HE2	1.71	0.56
1:N:170:THR:CG2	1:N:171:THR:H	2.15	0.56
2:B:338:ARG:HG3	2:B:338:ARG:NH1	2.21	0.56
2:O:27:THR:CG2	2:O:28:LYS:N	2.69	0.56
3:P:61:SER:O	3:P:62:LEU:HD23	2.06	0.56
2:B:23:ASP:OD1	2:B:24:LEU:N	2.39	0.56
6:S:100:GLU:O	6:S:103:GLU:HB3	2.05	0.56
5:E:131:GLU:H	5:E:131:GLU:CD	2.09	0.55
1:A:336:PHE:CE2	3:C:4:ASN:HB3	2.41	0.55
2:B:47:ILE:HD13	2:B:120:MET:HE2	1.88	0.55
5:R:29:SER:HA	5:R:32:ARG:HH21	1.71	0.55
2:O:407:SER:O	2:O:411:VAL:HG23	2.06	0.55
5:R:104:ALA:HA	5:R:107:ASN:ND2	2.22	0.55
6:S:58:ARG:HG3	6:S:89:TYR:OH	2.06	0.55
2:B:306:PRO:HB3	9:I:52:ARG:N	2.21	0.55
1:N:281:ASP:OD2	9:V:33:UNK:HB1	2.07	0.55
6:F:104:ARG:HA	2:O:83:PHE:CE2	2.41	0.55
8:U:21:ARG:HG3	8:U:21:ARG:HH11	1.71	0.55
3:C:6:ARG:HG2	3:C:16:ASN:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:257:VAL:HG22	2:B:424:MET:HG3	1.89	0.55
5:E:133:VAL:HG13	5:E:133:VAL:O	2.06	0.55
3:P:198:LEU:HD21	11:P:502:HEM:HMA3	1.88	0.55
1:A:327:ASP:HB3	1:A:328:PRO:HD2	1.87	0.55
3:P:247:SER:OG	3:P:250:LEU:HB2	2.07	0.55
5:E:130:PRO:HG2	5:E:131:GLU:OE2	2.06	0.55
3:P:125:MET:HE1	12:P:3001:IKR:I1	2.75	0.55
2:O:325:TYR:CD1	9:V:60:ALA:N	2.75	0.55
2:O:291:VAL:HA	2:O:297:GLN:NE2	2.21	0.55
4:D:62:LYS:O	4:D:66:GLU:HG3	2.05	0.55
1:N:61:HIS:CE1	1:N:134:ILE:HG12	2.41	0.55
1:A:117:VAL:HG23	1:A:118:GLN:H	1.70	0.55
1:N:146:THR:HG23	1:N:323:HIS:CE1	2.42	0.55
2:O:306:PRO:CG	9:V:51:CYS:HA	2.37	0.55
1:A:276:ILE:HG12	1:A:357:ALA:HB2	1.89	0.55
1:A:49:ASN:ND2	1:A:51:LYS:H	2.05	0.55
3:C:377:MET:CE	6:F:20:TYR:HB2	2.32	0.55
5:E:147:ILE:O	5:E:156:TYR:HA	2.06	0.55
2:O:394:ALA:HB3	2:O:397:VAL:HG23	1.88	0.55
4:D:229:VAL:CG2	7:G:20:PRO:HG3	2.37	0.55
1:N:85:HIS:HB2	1:N:100:LYS:HB2	1.89	0.55
4:Q:211:ILE:HG12	10:W:35:PHE:CZ	2.42	0.55
1:N:67:THR:HG21	1:N:115:ASP:OD2	2.07	0.55
9:V:72:ALA:HB1	9:V:73:PRO:CD	2.37	0.55
8:U:43:ARG:O	8:U:47:ARG:HG3	2.06	0.55
3:C:236:MET:O	3:C:239:PRO:HD2	2.06	0.55
1:N:424:ALA:HB1	1:N:428:ILE:HG21	1.89	0.55
5:E:52:LYS:HD3	5:E:52:LYS:C	2.27	0.55
7:T:29:ILE:O	7:T:34:LEU:HG	2.07	0.55
2:O:402:ILE:HD13	2:O:402:ILE:O	2.06	0.55
3:C:49:GLY:C	11:C:501:HEM:HAC	2.26	0.55
4:Q:62:LYS:O	4:Q:66:GLU:HG3	2.07	0.55
4:Q:75:ASP:OD2	4:Q:79:GLU:HB2	2.07	0.55
3:P:278:ALA:HB1	3:P:295:LEU:CD1	2.37	0.55
4:D:97:ASN:HB2	4:D:99:GLU:OE1	2.06	0.55
1:A:178:THR:CG2	1:A:179:ARG:N	2.69	0.55
3:C:377:MET:HE2	6:F:20:TYR:CB	2.33	0.55
2:O:56:ARG:HG3	2:O:56:ARG:NH1	2.22	0.55
3:P:219:ILE:HB	3:P:224:TYR:HD1	1.72	0.55
1:N:433:ASP:OD2	1:N:435:ASN:HB2	2.07	0.55
1:A:40:TRP:CZ3	1:A:198:ALA:HB3	2.43	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:63:ALA:O	1:N:116:VAL:HG13	2.07	0.54
1:A:281:ASP:OD2	1:A:284:PHE:HE1	1.90	0.54
2:B:357:VAL:O	2:B:361:LYS:HG3	2.06	0.54
5:R:133:VAL:HG13	5:R:133:VAL:O	2.07	0.54
8:H:28:GLU:O	8:H:32:LYS:HG3	2.07	0.54
10:J:14:PHE:CD2	10:J:14:PHE:N	2.71	0.54
4:Q:139:ALA:HB3	8:U:54:CYS:SG	2.47	0.54
1:N:61:HIS:NE2	2:O:287:ARG:NE	2.55	0.54
5:R:186:GLN:HE21	5:R:188:VAL:HG13	1.71	0.54
1:A:106:MET:HE2	1:A:107:PRO:HA	1.87	0.54
4:Q:102:ARG:NH1	4:Q:107:GLY:O	2.39	0.54
2:B:28:LYS:O	2:B:29:LEU:O	2.25	0.54
4:D:218:LEU:HD11	5:E:42:THR:HG22	1.89	0.54
3:P:222:HIS:HA	3:P:226:SER:OG	2.06	0.54
5:E:127:VAL:CG1	5:E:128:LYS:H	1.99	0.54
1:A:281:ASP:CG	9:I:33:UNK:HB2	2.28	0.54
1:N:58:PHE:HB3	1:N:182:LEU:HD21	1.88	0.54
1:A:61:HIS:CE1	1:A:134:ILE:HG12	2.42	0.54
2:B:402:ILE:HD13	2:B:402:ILE:C	2.27	0.54
7:G:59:TYR:O	7:G:63:THR:HB	2.07	0.54
5:E:155:GLY:HA3	5:E:166:ASP:O	2.08	0.54
1:N:395:TRP:HE3	1:N:395:TRP:HA	1.71	0.54
2:B:140:LEU:C	2:B:142:PRO:HD2	2.28	0.54
4:D:65:ALA:O	4:D:85:GLY:HA3	2.07	0.54
1:N:417:ASP:O	1:N:438:ARG:NH2	2.40	0.54
4:Q:116:ILE:HG23	4:Q:117:VAL:N	2.23	0.54
4:Q:232:SER:HB3	7:T:23:GLN:HE22	1.72	0.54
3:P:151:PHE:HB2	3:P:162:VAL:HG22	1.88	0.54
6:F:67:ASP:HA	6:F:70:LEU:HD23	1.90	0.54
5:E:109:GLU:HB2	5:E:167:ALA:HB3	1.89	0.54
2:O:56:ARG:HG3	2:O:171:ALA:HB1	1.89	0.54
3:P:6:ARG:HG2	3:P:16:ASN:HB2	1.90	0.54
2:O:181:TYR:CE1	2:O:182:ARG:CG	2.90	0.54
2:B:105:MET:HE2	2:B:107:TYR:HE1	1.72	0.54
1:N:369:LEU:HD12	1:N:392:LEU:HD11	1.88	0.54
4:D:37:CYS:C	4:D:39:ALA:H	2.09	0.54
5:E:171:ILE:HG22	5:E:179:ASN:OD1	2.08	0.54
7:G:50:PRO:HB2	7:G:51:PRO:HD3	1.89	0.54
1:N:178:THR:CG2	1:N:179:ARG:N	2.70	0.54
4:Q:57:THR:HG22	4:Q:58:GLU:N	2.23	0.54
3:C:120:LEU:HD13	11:C:502:HEM:CAB	2.35	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:153:PHE:HE2	5:E:172:ARG:HH21	1.56	0.54
3:C:142:TRP:O	3:C:146:VAL:HG23	2.08	0.54
3:P:23:PRO:HG3	7:T:4:PHE:CD1	2.43	0.54
2:O:162:ASN:O	2:O:244:ILE:HD12	2.08	0.54
8:H:35:GLU:O	8:H:39:LEU:HG	2.08	0.54
3:P:155:PRO:O	3:P:156:TYR:HB2	2.08	0.54
5:R:141:HIS:HB3	19:R:501:FES:S2	2.48	0.54
2:B:56:ARG:HG3	2:B:56:ARG:NH1	2.22	0.54
5:R:178:TYR:N	5:R:178:TYR:CD1	2.75	0.54
8:U:27:THR:HG22	8:U:29:LYS:H	1.73	0.54
2:B:365:LYS:O	2:B:369:LEU:HG	2.08	0.54
3:C:332:ASN:ND2	3:C:358:SER:OG	2.41	0.54
1:N:362:ARG:O	1:N:365:MET:HG2	2.07	0.54
5:E:130:PRO:HG2	5:E:131:GLU:H	1.73	0.54
9:I:63:ASP:CG	9:I:64:LEU:H	2.12	0.54
2:O:168:TYR:CE2	2:O:172:LEU:HD12	2.43	0.54
1:A:342:TRP:O	1:A:345:LEU:HB2	2.08	0.54
1:N:269:VAL:HG22	1:N:406:MET:HE2	1.89	0.54
5:R:86:ASN:HB2	5:R:99:ARG:HE	1.72	0.54
5:R:95:PRO:HG2	5:R:145:VAL:HG11	1.89	0.54
9:I:63:ASP:O	9:I:64:LEU:HB2	2.07	0.53
2:B:31:ASN:N	2:B:31:ASN:ND2	2.54	0.53
1:A:242:ARG:O	7:G:14:ILE:HA	2.07	0.53
4:D:116:ILE:HG23	4:D:117:VAL:N	2.22	0.53
1:N:37:VAL:HG12	1:N:199:ALA:CB	2.38	0.53
9:I:49:LEU:O	9:I:50:LEU:HD23	2.09	0.53
9:I:55:MET:O	9:I:58:ARG:HB2	2.07	0.53
5:R:148:ALA:O	5:R:149:ASN:HB2	2.09	0.53
2:B:312:PHE:HE1	9:I:62:ARG:O	1.91	0.53
2:O:46:ARG:O	2:O:46:ARG:HG3	2.07	0.53
8:U:34:ARG:HD2	8:U:38:GLU:OE2	2.09	0.53
2:B:207:VAL:HG21	2:B:383:GLY:CA	2.37	0.53
5:E:29:SER:HA	5:E:32:ARG:HH21	1.74	0.53
1:N:351:GLU:O	1:N:354:VAL:HG22	2.08	0.53
6:F:67:ASP:CG	6:F:71:LYS:HZ3	2.11	0.53
3:P:40:VAL:HA	3:P:43:MET:CE	2.38	0.53
1:N:239:SER:HB2	7:T:17:SER:O	2.08	0.53
2:O:130:PRO:HB2	2:O:132:PHE:CE2	2.43	0.53
1:A:307:PHE:C	1:A:307:PHE:CD1	2.81	0.53
5:E:119:ASP:HB3	5:E:179:ASN:ND2	2.23	0.53
2:B:305:GLN:HB3	2:B:306:PRO:HD2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:78:LEU:HB2	5:R:191:ASP:HA	1.91	0.53
2:B:312:PHE:CE1	9:I:62:ARG:O	2.61	0.53
2:O:247:GLN:HE22	2:O:429:ASP:HA	1.72	0.53
1:A:102:LEU:HD13	1:A:105:ASP:OD2	2.09	0.53
2:O:132:PHE:CD1	2:O:191:LEU:HB3	2.43	0.53
1:A:67:THR:HG21	1:A:115:ASP:OD2	2.09	0.53
5:R:76:ILE:O	5:R:193:VAL:HG12	2.08	0.53
2:B:248:ASN:HD22	2:B:249:GLY:N	2.06	0.53
4:Q:26:VAL:HG12	4:Q:55:THR:HG21	1.90	0.53
2:B:359:LYS:O	2:B:363:GLN:HG3	2.07	0.53
2:B:110:GLU:O	2:B:111:CYS:HB3	2.09	0.53
5:R:126:ARG:NH2	5:R:169:GLY:O	2.40	0.53
3:C:219:ILE:HB	3:C:224:TYR:CD1	2.43	0.53
8:U:52:GLU:HG3	8:U:53:GLN:N	2.24	0.53
1:N:32:GLN:OE1	2:O:373:GLU:HG2	2.08	0.53
3:C:23:PRO:HG3	7:G:4:PHE:CE1	2.44	0.53
1:A:7:THR:O	1:A:11:ILE:HG13	2.09	0.53
2:O:140:LEU:C	2:O:142:PRO:HD2	2.29	0.53
6:F:53:ASP:OD1	6:F:54:LEU:N	2.42	0.53
4:Q:235:MET:CE	6:S:64:ARG:HA	2.39	0.53
3:C:34:PHE:HB2	20:C:381:HOH:O	2.08	0.53
4:Q:28:ARG:HD2	4:Q:171:TYR:CD1	2.44	0.53
2:O:47:ILE:HD13	2:O:120:MET:HE1	1.88	0.53
4:Q:147:LEU:C	4:Q:148:HIS:HD2	2.13	0.53
5:E:163:SER:HA	5:E:174:GLY:HA3	1.90	0.53
5:R:98:VAL:HG22	5:R:134:ILE:HG12	1.90	0.53
2:O:221:GLU:HG3	2:O:222:GLN:N	2.24	0.53
2:O:248:ASN:C	2:O:248:ASN:ND2	2.59	0.53
1:A:145:MET:HB3	1:A:252:HIS:CD2	2.44	0.53
5:R:79:SER:OG	5:R:191:ASP:HB2	2.08	0.52
1:A:117:VAL:HG23	1:A:118:GLN:HG3	1.90	0.52
4:Q:220:TYR:CE2	14:Q:3003:CDL:H722	2.44	0.52
2:B:70:ARG:HG3	2:B:98:VAL:CG1	2.39	0.52
7:G:48:VAL:O	7:G:51:PRO:HD2	2.10	0.52
3:C:230:ILE:HG22	4:D:219:LEU:HD13	1.91	0.52
1:N:276:ILE:HG12	1:N:357:ALA:HB2	1.90	0.52
4:D:43:MET:HE1	4:D:189:PHE:CZ	2.44	0.52
2:O:273:SER:O	2:O:276:GLN:HB3	2.09	0.52
2:B:291:VAL:HA	2:B:297:GLN:NE2	2.24	0.52
2:B:239:TYR:HD1	2:B:260:GLU:OE1	1.91	0.52
3:C:20:ILE:HG22	3:C:21:ASP:OD1	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:162:VAL:C	3:C:164:TRP:H	2.12	0.52
4:Q:16:GLY:CA	4:Q:19:SER:OG	2.57	0.52
6:F:42:ASP:OD1	6:F:101:ARG:NH1	2.43	0.52
3:C:285:ILE:HB	3:C:291:GLY:HA2	1.90	0.52
2:B:209:ILE:HD13	2:B:378:LEU:HD23	1.91	0.52
10:W:57:HIS:CE1	10:W:58:LYS:HG3	2.44	0.52
2:B:333:ALA:O	2:B:337:ILE:HG13	2.09	0.52
2:B:247:GLN:HE22	2:B:429:ASP:HA	1.74	0.52
4:D:75:ASP:OD2	4:D:79:GLU:HB2	2.09	0.52
2:B:172:LEU:HD13	2:B:316:TYR:CD1	2.45	0.52
3:P:208:ASN:HB2	3:P:209:PRO:HD2	1.90	0.52
3:C:9:HIS:CD2	3:C:11:LEU:H	2.27	0.52
2:B:303:THR:HA	2:B:335:GLU:OE1	2.08	0.52
10:J:57:HIS:CE1	10:J:58:LYS:HG3	2.44	0.52
6:S:12:LEU:C	6:S:14:ASP:H	2.12	0.52
4:Q:12:TRP:NE1	4:Q:125:ASP:OD2	2.34	0.52
7:T:28:ASN:HB2	7:T:32:ASP:HB3	1.91	0.52
2:O:274:VAL:O	2:O:278:VAL:HG23	2.10	0.52
3:C:279:TYR:O	3:C:283:ARG:HG3	2.09	0.52
3:P:287:ASN:O	3:P:288:LYS:C	2.46	0.52
3:P:9:HIS:CD2	3:P:12:LEU:H	2.27	0.52
1:N:106:MET:HG3	1:N:203:ILE:CD1	2.38	0.52
2:B:25:GLU:HB2	2:B:213:HIS:ND1	2.24	0.52
1:N:7:THR:O	1:N:11:ILE:HG13	2.10	0.52
2:B:71:LEU:CD2	9:I:68:ILE:HG13	2.40	0.52
2:O:303:THR:HA	2:O:335:GLU:OE1	2.09	0.52
5:E:58:PHE:O	5:E:61:SER:HB3	2.09	0.52
3:C:287:ASN:O	3:C:288:LYS:C	2.48	0.52
5:E:95:PRO:HG2	5:E:145:VAL:HG11	1.90	0.52
2:O:76:THR:HG22	2:O:81:SER:HA	1.92	0.52
5:E:84:GLY:CA	5:E:102:THR:HG23	2.39	0.52
5:E:130:PRO:HG2	5:E:131:GLU:CD	2.31	0.52
5:R:76:ILE:HD12	5:R:98:VAL:HG21	1.91	0.52
1:N:117:VAL:HG23	1:N:118:GLN:H	1.74	0.52
1:N:133:VAL:O	1:N:137:GLU:HG3	2.10	0.52
2:O:18:CYS:HB2	2:O:19:PRO:HD3	1.92	0.52
6:S:31:LEU:HD21	6:S:65:ALA:CB	2.40	0.52
2:O:105:MET:HE2	2:O:107:TYR:HE1	1.75	0.52
5:E:165:TYR:CE2	5:E:180:LEU:HG	2.45	0.52
3:C:23:PRO:HG3	7:G:4:PHE:CD1	2.45	0.52
2:O:156:GLN:NE2	9:V:77:ARG:C	2.63	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:9:HIS:CD2	3:C:12:LEU:H	2.27	0.52
2:O:96:LEU:HD12	2:O:97:SER:N	2.25	0.52
2:B:274:VAL:O	2:B:278:VAL:HG23	2.10	0.52
1:N:45:SER:HA	1:N:48:GLU:HG3	1.92	0.52
1:A:317:THR:HG23	1:A:318:GLY:N	2.25	0.52
7:T:50:PRO:HB2	7:T:51:PRO:HD3	1.92	0.52
1:N:23:LEU:HA	1:N:192:ALA:O	2.10	0.52
3:P:198:LEU:HD13	13:P:3002:UQ:HM53	1.92	0.52
8:H:28:GLU:HG2	8:H:32:LYS:HE3	1.91	0.52
3:C:92:PHE:O	3:C:95:ILE:HG22	2.10	0.52
8:H:21:ARG:O	8:H:25:GLU:HG3	2.10	0.52
6:S:77:LYS:HA	6:S:80:TRP:CE2	2.44	0.52
3:C:342:GLN:NE2	3:C:343:PRO:HD2	2.22	0.51
5:E:129:LYS:CB	5:E:132:TRP:HB2	2.40	0.51
2:B:47:ILE:HD11	2:B:116:VAL:CG1	2.39	0.51
2:O:305:GLN:HB3	2:O:306:PRO:HD2	1.92	0.51
8:U:35:GLU:O	8:U:39:LEU:HG	2.09	0.51
1:N:40:TRP:CD1	1:N:96:ALA:HB2	2.45	0.51
1:N:81:SER:HB3	2:O:359:LYS:HD3	1.93	0.51
3:P:120:LEU:HD13	11:P:502:HEM:HAB	1.91	0.51
1:N:281:ASP:HB3	9:V:33:UNK:HB2	1.91	0.51
3:C:246:PHE:C	3:C:248:PRO:HD3	2.30	0.51
3:C:365:ILE:O	3:C:368:PRO:HG2	2.09	0.51
6:S:58:ARG:HH11	6:S:58:ARG:HG3	1.76	0.51
5:R:169:GLY:O	5:R:179:ASN:HB3	2.11	0.51
1:N:4:TYR:HB2	2:O:114:ASP:OD1	2.11	0.51
7:T:49:ALA:HB3	7:T:50:PRO:HD3	1.91	0.51
2:O:170:THR:O	2:O:172:LEU:N	2.43	0.51
2:B:46:ARG:O	2:B:46:ARG:HG3	2.10	0.51
10:J:60:GLU:O	10:J:61:ALA:HB3	2.09	0.51
3:P:182:LEU:O	3:P:186:LEU:HG	2.10	0.51
5:E:189:GLY:O	5:E:192:LEU:O	2.28	0.51
1:N:354:VAL:HG23	1:N:355:LYS:N	2.26	0.51
6:F:58:ARG:HG3	6:F:89:TYR:OH	2.11	0.51
3:P:246:PHE:C	3:P:248:PRO:HD3	2.31	0.51
5:E:139:CYS:SG	5:E:176:ALA:HB2	2.50	0.51
2:O:424:MET:HB2	2:O:436:LEU:HD13	1.93	0.51
5:E:76:ILE:O	5:E:193:VAL:HG12	2.11	0.51
8:H:43:ARG:HD2	8:H:47:ARG:NH2	2.26	0.51
2:O:46:ARG:HG3	2:O:379:LEU:HD22	1.91	0.51
10:W:10:TYR:CE2	10:W:15:ARG:HD2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:106:MET:CG	1:N:203:ILE:HD13	2.39	0.51
1:A:133:VAL:O	1:A:137:GLU:HG3	2.10	0.51
2:B:215:ASP:O	2:B:219:VAL:HG23	2.11	0.51
4:D:57:THR:HG22	4:D:58:GLU:N	2.26	0.51
1:A:281:ASP:OD2	9:I:33:UNK:HG2	2.11	0.51
3:P:23:PRO:HG3	7:T:4:PHE:CE1	2.46	0.51
1:A:61:HIS:NE2	2:B:287:ARG:NE	2.59	0.51
4:Q:240:PRO:HD3	7:T:12:HIS:CE1	2.45	0.51
5:R:52:LYS:HD3	5:R:52:LYS:C	2.30	0.51
1:A:108:LYS:HG3	1:A:108:LYS:O	2.11	0.51
5:E:171:ILE:HG12	5:E:176:ALA:O	2.10	0.51
2:B:270:ASN:ND2	2:B:270:ASN:N	2.49	0.51
9:V:55:MET:HA	9:V:58:ARG:HG3	1.92	0.51
2:B:56:ARG:HA	2:B:171:ALA:O	2.11	0.51
3:P:342:GLN:NE2	3:P:343:PRO:HD2	2.22	0.51
2:O:325:TYR:CD1	9:V:60:ALA:CB	2.93	0.51
2:B:206:LEU:HD23	2:B:220:ALA:HB2	1.93	0.51
2:B:124:LEU:O	2:B:128:THR:HG23	2.10	0.51
5:E:109:GLU:CB	5:E:167:ALA:HB3	2.41	0.51
2:B:291:VAL:HA	2:B:297:GLN:HE21	1.75	0.51
1:A:23:LEU:HD23	1:A:24:ARG:N	2.26	0.51
3:C:5:ILE:O	3:C:5:ILE:HG22	2.11	0.51
2:B:372:VAL:O	2:B:372:VAL:HG12	2.11	0.51
8:U:36:ARG:NH1	8:U:36:ARG:HB3	2.26	0.51
4:Q:134:TYR:CG	4:Q:162:PRO:HG3	2.46	0.51
3:P:172:ASP:HB3	3:P:174:PRO:HD2	1.92	0.51
4:Q:237:TYR:HB2	6:S:60:PHE:CD1	2.46	0.51
5:R:165:TYR:CD2	5:R:180:LEU:HG	2.47	0.50
5:R:78:LEU:HD11	5:R:187:PHE:CE1	2.46	0.50
2:O:308:ASP:CG	9:V:56:SER:HA	2.31	0.50
2:O:279:LEU:O	2:O:295:LEU:HB3	2.11	0.50
1:A:75:PHE:O	1:A:79:VAL:HG23	2.11	0.50
1:A:146:THR:HG23	1:A:323:HIS:CE1	2.47	0.50
4:D:28:ARG:HD2	4:D:171:TYR:CD1	2.46	0.50
3:P:72:ARG:NE	4:Q:115:TYR:OH	2.44	0.50
3:P:92:PHE:HA	3:P:95:ILE:HG22	1.92	0.50
2:O:268:GLU:HG2	2:O:268:GLU:O	2.10	0.50
7:G:49:ALA:HB3	7:G:50:PRO:HD3	1.92	0.50
3:C:377:MET:HE1	6:F:20:TYR:CD1	2.47	0.50
2:O:286:LYS:HE2	2:O:287:ARG:CZ	2.40	0.50
2:B:21:ALA:O	2:B:22:GLU:CB	2.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:72:ALA:HB1	9:I:73:PRO:HD2	1.93	0.50
1:N:87:ASN:CG	1:N:88:GLY:H	2.14	0.50
2:O:26:ILE:O	2:O:26:ILE:HG12	2.10	0.50
4:Q:26:VAL:CG2	4:Q:188:THR:HG22	2.41	0.50
8:U:21:ARG:O	8:U:25:GLU:HG3	2.12	0.50
4:Q:235:MET:HE1	6:S:64:ARG:N	2.27	0.50
1:N:40:TRP:CZ3	1:N:198:ALA:HB3	2.46	0.50
4:Q:240:PRO:O	4:Q:241:LYS:OXT	2.29	0.50
4:Q:197:GLU:O	4:Q:198:HIS:C	2.50	0.50
8:U:28:GLU:HG2	8:U:32:LYS:HE3	1.93	0.50
10:W:58:LYS:HB2	10:W:59:TYR:CE1	2.46	0.50
4:Q:148:HIS:CD2	4:Q:148:HIS:N	2.79	0.50
6:S:32:MET:CE	6:S:87:LYS:H	2.23	0.50
2:B:258:VAL:CG2	2:B:321:LEU:HD22	2.41	0.50
4:D:197:GLU:O	4:D:198:HIS:C	2.50	0.50
1:A:438:ARG:HG3	1:A:438:ARG:HH11	1.77	0.50
1:A:395:TRP:HE3	1:A:395:TRP:HA	1.74	0.50
6:F:51:PRO:HD2	6:F:54:LEU:HD12	1.93	0.50
5:E:185:TYR:O	5:E:186:GLN:HB3	2.12	0.50
4:D:143:VAL:HG21	4:D:149:TYR:HB2	1.94	0.50
6:S:13:MET:CA	6:S:16:ILE:HB	2.41	0.50
3:C:172:ASP:HB3	3:C:174:PRO:HD2	1.93	0.50
4:D:26:VAL:CG2	4:D:188:THR:HG22	2.42	0.50
5:R:53:ASN:O	5:R:56:THR:HB	2.10	0.50
1:N:102:LEU:HD13	1:N:105:ASP:OD2	2.11	0.50
5:R:155:GLY:HA3	5:R:166:ASP:O	2.11	0.50
2:O:62:ASN:O	2:O:65:THR:CG2	2.57	0.50
4:Q:221:TYR:CE2	5:R:39:VAL:HG21	2.47	0.50
6:S:16:ILE:O	6:S:19:TRP:HB3	2.12	0.50
7:G:36:ASN:O	7:G:40:ARG:HG3	2.12	0.50
4:D:26:VAL:HG12	4:D:55:THR:HG21	1.93	0.50
3:P:162:VAL:C	3:P:164:TRP:H	2.14	0.50
1:A:344:ARG:HH22	1:A:353:GLU:CD	2.14	0.50
1:N:436:ARG:NH1	3:P:220:PRO:HB2	2.26	0.50
5:R:114:VAL:HG12	5:R:114:VAL:O	2.12	0.50
8:H:40:CYS:HA	8:H:43:ARG:NH1	2.27	0.50
1:N:106:MET:HE2	1:N:107:PRO:HA	1.92	0.50
4:D:105:ASN:O	4:D:106:ASN:HB2	2.12	0.50
1:A:158:PHE:O	1:A:164:ALA:HB2	2.12	0.50
4:Q:105:ASN:O	4:Q:106:ASN:HB2	2.11	0.50
3:C:271:PRO:HB2	3:C:275:PHE:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:34:LYS:O	4:Q:34:LYS:HG2	2.11	0.50
2:B:146:VAL:HG12	2:B:147:ASP:N	2.27	0.50
1:N:60:GLU:OE2	1:N:89:TYR:HA	2.11	0.50
5:E:84:GLY:N	5:E:102:THR:HG23	2.26	0.50
3:P:342:GLN:HB3	3:P:348:PHE:CD1	2.47	0.50
4:D:148:HIS:CD2	4:D:148:HIS:N	2.80	0.50
3:C:321:LEU:HB2	3:C:374:GLU:OE1	2.10	0.50
1:N:158:PHE:O	1:N:164:ALA:HB2	2.12	0.50
3:C:145:THR:O	3:C:149:ASN:HB2	2.12	0.50
3:P:184:PHE:O	3:P:184:PHE:HD2	1.95	0.50
4:D:223:LYS:HD3	4:D:223:LYS:C	2.32	0.50
9:I:32:UNK:N	9:I:73:PRO:CG	2.75	0.49
3:P:142:TRP:HB3	3:P:269:ILE:HD13	1.94	0.49
4:Q:109:LEU:O	4:Q:111:PRO:HD3	2.12	0.49
4:Q:203:ARG:HD3	18:Q:3009:BOG:O6	2.12	0.49
1:A:390:ILE:HG23	1:A:394:GLU:OE1	2.12	0.49
5:R:82:PRO:HG2	5:R:85:LYS:HB2	1.94	0.49
3:P:9:HIS:CD2	3:P:11:LEU:H	2.31	0.49
1:A:103:SER:HB3	1:A:202:GLY:O	2.12	0.49
2:O:31:ASN:ND2	2:O:31:ASN:N	2.60	0.49
1:N:117:VAL:HG23	1:N:118:GLN:HG3	1.94	0.49
2:O:67:HIS:O	2:O:70:ARG:HB3	2.13	0.49
4:Q:223:LYS:C	4:Q:223:LYS:HD3	2.32	0.49
2:B:181:TYR:CE1	2:B:182:ARG:CG	2.95	0.49
4:D:148:HIS:CE1	4:D:161:ALA:HB2	2.48	0.49
5:E:187:PHE:C	5:E:189:GLY:N	2.66	0.49
1:N:87:ASN:OD1	2:O:286:LYS:HD2	2.12	0.49
2:B:96:LEU:HB3	9:I:70:LEU:HD22	1.94	0.49
6:S:13:MET:HA	6:S:16:ILE:HD12	1.93	0.49
3:P:332:ASN:ND2	3:P:358:SER:OG	2.43	0.49
2:O:333:ALA:O	2:O:337:ILE:HG13	2.12	0.49
2:B:248:ASN:ND2	2:B:248:ASN:C	2.62	0.49
1:N:242:ARG:O	7:T:14:ILE:HA	2.12	0.49
4:Q:70:VAL:CG2	4:Q:83:ARG:CZ	2.90	0.49
4:Q:117:VAL:O	4:Q:123:GLY:HA2	2.12	0.49
1:A:23:LEU:HA	1:A:192:ALA:O	2.13	0.49
3:P:359:TYR:HD2	3:P:360:PHE:CD1	2.30	0.49
1:N:361:LEU:O	1:N:364:ALA:HB3	2.12	0.49
5:E:141:HIS:HB2	5:E:176:ALA:HA	1.94	0.49
5:E:84:GLY:N	5:E:100:HIS:O	2.40	0.49
5:E:98:VAL:HG22	5:E:134:ILE:HG12	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:37:VAL:HG12	1:N:199:ALA:HA	1.95	0.49
2:O:272:PHE:O	2:O:276:GLN:N	2.44	0.49
8:H:17:LEU:HD21	8:H:21:ARG:NH2	2.28	0.49
7:G:30:PHE:O	7:G:35:PRO:HD3	2.11	0.49
1:N:270:LEU:HD22	1:N:320:PHE:CE1	2.48	0.49
3:P:325:LEU:HD21	3:P:366:LEU:HB3	1.95	0.49
7:T:30:PHE:CD2	7:T:34:LEU:HD12	2.47	0.49
4:Q:181:GLN:CA	8:U:77:LEU:HD22	2.42	0.49
2:O:159:VAL:HG23	2:O:160:LEU:HD23	1.95	0.49
8:U:73:LEU:HD12	8:U:73:LEU:O	2.12	0.49
1:A:63:ALA:O	1:A:116:VAL:HG13	2.12	0.49
2:O:209:ILE:HD13	2:O:378:LEU:HD23	1.95	0.49
3:P:90:PHE:HE1	3:P:236:MET:HB3	1.77	0.49
1:A:293:ARG:HD3	1:A:344:ARG:NH1	2.27	0.49
1:N:293:ARG:O	1:N:297:LEU:HG	2.13	0.49
1:N:212:ALA:O	1:N:216:PHE:HB2	2.13	0.49
10:W:60:GLU:HG3	10:W:60:GLU:O	2.12	0.49
2:O:47:ILE:HD13	2:O:120:MET:HE2	1.93	0.49
2:O:306:PRO:HB3	9:V:52:ARG:N	2.27	0.49
1:A:37:VAL:HG12	1:A:199:ALA:HA	1.93	0.49
2:B:56:ARG:HG3	2:B:171:ALA:HB1	1.93	0.49
2:O:341:MET:CE	2:O:417:PHE:CE2	2.95	0.49
2:B:62:ASN:O	2:B:65:THR:CG2	2.60	0.49
3:C:172:ASP:C	3:C:174:PRO:HD2	2.32	0.49
2:B:325:TYR:HD1	9:I:60:ALA:CB	2.26	0.49
2:O:71:LEU:CD1	2:O:144:LEU:HD23	2.43	0.49
8:H:21:ARG:HG3	8:H:21:ARG:HH11	1.77	0.49
1:A:161:THR:HG21	1:A:235:ARG:H	1.78	0.49
2:O:29:LEU:HB3	2:O:30:PRO:CD	2.43	0.49
2:B:286:LYS:HE2	2:B:287:ARG:HH12	1.78	0.49
2:O:47:ILE:HD11	2:O:116:VAL:CG1	2.42	0.49
3:C:90:PHE:HE1	3:C:236:MET:HB3	1.77	0.49
3:C:208:ASN:HB2	3:C:209:PRO:HD2	1.95	0.49
2:O:71:LEU:HD11	2:O:144:LEU:HD23	1.95	0.49
2:B:73:SER:OG	2:B:74:PRO:HD3	2.13	0.49
1:N:10:ASN:OD1	2:O:19:PRO:HD2	2.13	0.49
4:D:235:MET:HE2	6:F:64:ARG:HA	1.94	0.49
1:N:223:TYR:HD2	1:N:223:TYR:H	1.61	0.49
2:B:150:VAL:CG2	2:B:151:ALA:N	2.76	0.48
6:S:96:GLU:OE1	6:S:99:ARG:NH2	2.46	0.48
1:A:23:LEU:HB2	1:A:192:ALA:HB1	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:TYR:HD2	1:A:223:TYR:H	1.60	0.48
3:P:285:ILE:HB	3:P:291:GLY:HA2	1.95	0.48
1:A:138:LEU:HD21	1:A:168:GLU:HB3	1.94	0.48
8:U:44:VAL:HG21	8:U:54:CYS:SG	2.53	0.48
4:D:57:THR:HB	4:D:60:GLU:HG3	1.93	0.48
2:B:147:ASP:O	2:B:150:VAL:HG22	2.13	0.48
2:O:62:ASN:ND2	2:O:65:THR:HG21	2.28	0.48
1:A:206:LYS:HA	1:A:209:VAL:HG12	1.95	0.48
4:D:70:VAL:CG2	4:D:83:ARG:CZ	2.91	0.48
2:B:46:ARG:CD	2:B:110:GLU:HG2	2.44	0.48
1:A:15:ASN:O	1:A:26:ALA:HA	2.13	0.48
7:T:59:TYR:O	7:T:63:THR:HB	2.14	0.48
3:P:125:MET:HE2	3:P:275:PHE:HE2	1.79	0.48
5:E:78:LEU:HB3	5:E:132:TRP:CZ2	2.48	0.48
3:P:70:THR:HA	3:P:74:VAL:CG2	2.43	0.48
8:H:10:GLU:C	8:H:11:GLU:HG3	2.34	0.48
3:C:106:GLY:HA2	3:C:108:TYR:CE2	2.47	0.48
4:Q:35:GLN:NE2	4:Q:169:LEU:HD12	2.28	0.48
1:A:354:VAL:HG23	1:A:355:LYS:N	2.28	0.48
3:C:2:ALA:HB1	3:C:3:PRO:HD2	1.96	0.48
7:T:46:PHE:O	7:T:50:PRO:HG2	2.13	0.48
4:Q:195:GLU:OE1	4:Q:201:ARG:NH2	2.45	0.48
3:C:207:ASN:ND2	3:C:208:ASN:H	2.11	0.48
2:B:24:LEU:O	2:B:24:LEU:HG	2.13	0.48
8:U:34:ARG:HB2	8:U:61:PHE:CE1	2.48	0.48
1:A:37:VAL:HG12	1:A:199:ALA:CB	2.43	0.48
4:Q:37:CYS:C	4:Q:39:ALA:H	2.17	0.48
2:O:345:LYS:O	2:O:349:GLN:HG3	2.13	0.48
3:P:311:SER:HB2	3:P:319:ARG:NH1	2.28	0.48
8:U:48:SER:O	8:U:49:HIS:ND1	2.45	0.48
1:N:108:LYS:O	1:N:108:LYS:HG3	2.12	0.48
3:P:271:PRO:HD2	3:P:279:TYR:CD2	2.48	0.48
2:B:200:THR:OG1	2:B:203:ARG:HD3	2.14	0.48
2:O:287:ARG:HA	9:V:53:GLU:HG3	1.95	0.48
2:O:46:ARG:CD	2:O:110:GLU:HG2	2.44	0.48
1:A:18:THR:HG23	1:A:24:ARG:HG3	1.94	0.48
10:J:10:TYR:CE2	10:J:15:ARG:HD2	2.48	0.48
3:P:5:ILE:O	3:P:5:ILE:HG22	2.14	0.48
2:B:168:TYR:HE2	2:B:172:LEU:HD12	1.77	0.48
2:B:306:PRO:HA	9:I:52:ARG:HG2	1.96	0.48
2:B:286:LYS:HE2	2:B:287:ARG:CZ	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:344:LEU:HD13	2:B:417:PHE:CE2	2.48	0.48
6:F:58:ARG:HH11	6:F:58:ARG:HG3	1.77	0.48
10:J:40:ASP:O	10:J:44:GLU:HG3	2.13	0.48
1:A:38:GLY:HA3	1:A:98:TYR:HA	1.95	0.48
5:E:77:LYS:HE2	5:E:79:SER:OG	2.14	0.48
3:C:166:TRP:HA	3:C:175:THR:HG23	1.96	0.48
4:Q:97:ASN:HB2	4:Q:99:GLU:OE1	2.13	0.48
4:D:34:LYS:O	4:D:34:LYS:HG2	2.12	0.48
5:E:161:HIS:HB2	19:E:501:FES:S1	2.54	0.48
4:D:47:ALA:N	4:D:50:ASN:HD22	2.03	0.48
6:S:99:ARG:HB3	6:S:99:ARG:HH11	1.78	0.48
2:O:166:ALA:HB1	2:O:242:GLY:C	2.34	0.48
2:B:290:SER:O	2:B:297:GLN:HG2	2.14	0.48
2:B:273:SER:O	2:B:276:GLN:HB3	2.13	0.48
2:O:193:HIS:O	2:O:197:ASN:ND2	2.46	0.48
2:O:37:SER:HB3	2:O:213:HIS:CG	2.48	0.48
5:R:178:TYR:N	5:R:178:TYR:HD1	2.11	0.48
1:A:170:THR:CG2	1:A:171:THR:H	2.23	0.48
2:B:144:LEU:HB2	2:B:183:ILE:HD12	1.96	0.48
8:U:17:LEU:HD21	8:U:21:ARG:NH2	2.29	0.48
4:D:37:CYS:C	4:D:39:ALA:N	2.67	0.48
3:C:142:TRP:HB3	3:C:269:ILE:HD13	1.95	0.48
1:N:40:TRP:CZ2	1:N:377:GLU:HA	2.49	0.48
1:N:15:ASN:O	1:N:26:ALA:HA	2.14	0.48
1:A:270:LEU:HD22	1:A:320:PHE:CE1	2.49	0.48
6:S:53:ASP:OD1	6:S:54:LEU:N	2.46	0.48
1:A:53:ASN:N	1:A:173:ASN:HD22	2.11	0.48
1:A:69:LYS:HD2	1:A:70:ARG:NH2	2.23	0.48
3:C:9:HIS:HB3	3:C:12:LEU:HB2	1.95	0.48
8:H:34:ARG:HB2	8:H:61:PHE:CE1	2.49	0.48
5:E:121:GLN:CG	5:E:170:ARG:HD3	2.18	0.47
2:B:314:VAL:CG1	9:I:63:ASP:HB3	2.39	0.47
3:P:138:GLN:O	3:P:142:TRP:HD1	1.97	0.47
7:T:30:PHE:O	7:T:35:PRO:HD3	2.14	0.47
2:O:357:VAL:CG1	2:O:361:LYS:HE3	2.44	0.47
3:C:350:ILE:CG2	3:C:351:ILE:N	2.77	0.47
3:P:132:TYR:O	3:P:135:PRO:HD2	2.14	0.47
1:N:94:GLN:NE2	1:N:381:SER:OG	2.37	0.47
4:D:16:GLY:CA	4:D:19:SER:OG	2.62	0.47
1:N:382:HIS:HB3	1:N:388:ARG:O	2.13	0.47
6:F:71:LYS:O	6:F:72:HIS:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:150:VAL:CG2	2:O:151:ALA:N	2.77	0.47
5:R:78:LEU:HD13	5:R:132:TRP:HE1	1.76	0.47
7:G:81:GLN:HG3	7:G:81:GLN:OXT	2.13	0.47
5:E:178:TYR:CD1	5:E:178:TYR:N	2.82	0.47
2:O:133:ARG:HD3	2:O:135:TRP:CZ2	2.48	0.47
2:B:159:VAL:HG23	2:B:160:LEU:HD23	1.96	0.47
4:D:134:TYR:CG	4:D:162:PRO:HG3	2.49	0.47
1:N:53:ASN:N	1:N:173:ASN:HD22	2.12	0.47
3:P:261:ASN:HD21	3:P:264:VAL:HG23	1.78	0.47
4:Q:218:LEU:CD1	5:R:42:THR:HG22	2.44	0.47
4:Q:117:VAL:HG21	4:Q:191:ARG:HA	1.95	0.47
4:D:117:VAL:HG21	4:D:191:ARG:HA	1.96	0.47
2:O:146:VAL:HG12	2:O:147:ASP:N	2.28	0.47
5:E:82:PRO:O	5:E:100:HIS:HB3	2.14	0.47
3:C:342:GLN:HB3	3:C:348:PHE:CD1	2.49	0.47
1:A:170:THR:CG2	1:A:171:THR:N	2.78	0.47
2:O:156:GLN:HE22	9:V:77:ARG:C	2.18	0.47
2:B:47:ILE:HD13	2:B:120:MET:HE1	1.96	0.47
3:C:31:TRP:O	3:C:101:ARG:HG3	2.14	0.47
2:B:279:LEU:O	2:B:295:LEU:HB3	2.13	0.47
2:O:122:TYR:O	2:O:126:VAL:HG23	2.15	0.47
2:O:225:ASN:O	2:O:227:ARG:HG2	2.15	0.47
4:Q:2:GLU:O	4:Q:3:LEU:O	2.31	0.47
4:Q:65:ALA:O	4:Q:85:GLY:HA3	2.14	0.47
3:C:37:LEU:HD21	3:C:233:LEU:HA	1.95	0.47
1:A:102:LEU:H	1:A:102:LEU:CD1	2.10	0.47
2:B:157:VAL:O	2:B:157:VAL:HG22	2.14	0.47
2:O:341:MET:HE3	2:O:417:PHE:HE2	1.74	0.47
5:R:95:PRO:HG2	5:R:145:VAL:CG1	2.45	0.47
3:P:182:LEU:HA	3:P:182:LEU:HD23	1.58	0.47
10:J:44:GLU:OE2	10:J:53:LYS:NZ	2.42	0.47
2:O:259:THR:OG1	2:O:422:LYS:HG3	2.14	0.47
2:B:57:TYR:HD1	2:B:57:TYR:N	2.11	0.47
1:N:87:ASN:CG	1:N:88:GLY:N	2.68	0.47
2:B:286:LYS:HE2	2:B:287:ARG:NH2	2.29	0.47
2:B:243:GLU:OE1	2:B:436:LEU:HB3	2.14	0.47
2:B:162:ASN:O	2:B:244:ILE:HD12	2.15	0.47
2:O:43:PRO:O	2:O:113:ARG:HG3	2.13	0.47
3:P:350:ILE:HG23	3:P:351:ILE:N	2.29	0.47
2:B:122:TYR:O	2:B:126:VAL:HG23	2.15	0.47
4:D:109:LEU:O	4:D:111:PRO:HD3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:150:ASN:O	4:Q:156:GLN:HA	2.14	0.47
6:S:71:LYS:O	6:S:72:HIS:HB2	2.14	0.47
2:O:372:VAL:O	2:O:372:VAL:HG12	2.14	0.47
5:R:101:ARG:HA	5:R:105:GLU:OE1	2.15	0.47
2:O:63:LEU:HB2	2:O:182:ARG:CD	2.40	0.47
8:H:44:VAL:HG13	8:H:50:THR:HG21	1.95	0.47
1:N:23:LEU:HB2	1:N:192:ALA:HB1	1.97	0.47
2:O:290:SER:O	2:O:297:GLN:HG2	2.15	0.47
2:B:83:PHE:CE2	6:S:104:ARG:HA	2.49	0.47
2:O:110:GLU:O	2:O:111:CYS:HB3	2.13	0.47
3:P:321:LEU:HB2	3:P:374:GLU:OE1	2.15	0.47
4:D:203:ARG:HD3	18:D:2009:BOG:O6	2.15	0.47
3:C:325:LEU:HD21	3:C:366:LEU:HB3	1.97	0.47
1:N:75:PHE:O	1:N:79:VAL:HG23	2.14	0.47
3:P:16:ASN:OD1	3:P:21:ASP:OD1	2.32	0.47
3:P:30:ALA:HB1	14:Q:3003:CDL:H111	1.97	0.47
1:N:10:ASN:OD1	2:O:18:CYS:N	2.47	0.47
1:A:147:ASN:C	1:A:149:THR:N	2.68	0.47
5:R:185:TYR:CD2	5:R:185:TYR:N	2.83	0.47
1:N:46:ARG:HD3	1:N:231:LEU:HD13	1.95	0.47
2:O:73:SER:OG	2:O:74:PRO:HD3	2.15	0.47
3:C:151:PHE:HB2	3:C:162:VAL:CG2	2.44	0.47
1:N:40:TRP:CD2	1:N:380:GLY:HA3	2.50	0.47
1:A:244:ARG:NE	7:G:10:VAL:HB	2.29	0.47
1:A:439:SER:HA	1:A:442:TYR:CE2	2.49	0.47
3:P:133:VAL:HG22	3:P:144:ALA:HB2	1.96	0.47
3:C:182:LEU:O	3:C:186:LEU:HG	2.15	0.47
7:T:48:VAL:HG12	7:T:49:ALA:N	2.30	0.47
1:A:180:ALA:O	1:A:183:ALA:HB3	2.15	0.47
5:R:185:TYR:HD2	5:R:185:TYR:N	2.12	0.47
1:N:69:LYS:HD2	1:N:70:ARG:NH2	2.22	0.47
3:C:202:HIS:NE2	13:C:2002:UQ:O4	2.44	0.47
9:V:63:ASP:OD1	9:V:63:ASP:N	2.48	0.47
3:C:164:TRP:CZ2	5:R:62:LEU:HD12	2.50	0.47
2:B:86:THR:O	2:B:90:GLU:HG3	2.14	0.47
2:B:345:LYS:O	2:B:349:GLN:HG3	2.15	0.47
4:D:240:PRO:O	4:D:241:LYS:C	2.53	0.47
10:W:20:PHE:O	10:W:24:VAL:HG23	2.15	0.47
2:B:353:THR:HB	2:B:356:ASP:CG	2.35	0.46
1:N:180:ALA:O	1:N:183:ALA:HB3	2.15	0.46
5:R:100:HIS:CD2	5:R:131:GLU:HB2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:9:HIS:HB3	3:P:12:LEU:HB2	1.98	0.46
2:O:239:TYR:HE2	2:O:241:GLY:HA2	1.79	0.46
2:B:277:HIS:NE2	2:B:364:LEU:HD13	2.30	0.46
2:O:290:SER:C	2:O:297:GLN:HE21	2.19	0.46
8:U:21:ARG:HG3	8:U:21:ARG:NH1	2.29	0.46
3:P:212:ILE:HD12	6:S:62:ILE:HG23	1.97	0.46
3:P:230:ILE:HG22	4:Q:219:LEU:HD13	1.97	0.46
1:A:7:THR:HG21	2:B:113:ARG:CD	2.43	0.46
5:E:163:SER:H	5:E:175:PRO:HD2	1.79	0.46
1:N:140:GLU:OE2	9:V:50:LEU:N	2.45	0.46
2:O:424:MET:HG2	2:O:425:ALA:H	1.79	0.46
3:C:198:LEU:HD21	11:C:502:HEM:CMA	2.45	0.46
5:R:83:GLU:HG2	5:R:100:HIS:CD2	2.51	0.46
3:P:172:ASP:C	3:P:174:PRO:HD2	2.36	0.46
3:P:40:VAL:O	3:P:44:THR:OG1	2.33	0.46
1:N:146:THR:O	1:N:150:PHE:HD1	1.98	0.46
4:D:43:MET:CE	4:D:189:PHE:CZ	2.98	0.46
4:D:235:MET:CE	6:F:64:ARG:HA	2.45	0.46
4:Q:238:ARG:CZ	5:R:5:VAL:HG22	2.45	0.46
3:C:359:TYR:HD2	3:C:360:PHE:CD1	2.33	0.46
2:O:353:THR:HB	2:O:356:ASP:OD1	2.15	0.46
7:G:48:VAL:HG12	7:G:49:ALA:N	2.31	0.46
3:P:6:ARG:HG2	3:P:16:ASN:CB	2.45	0.46
2:B:239:TYR:C	2:B:239:TYR:CD2	2.88	0.46
2:O:47:ILE:HG22	2:O:48:GLY:N	2.29	0.46
1:N:249:PRO:HG2	1:N:250:VAL:N	2.31	0.46
4:Q:235:MET:HE1	6:S:63:LYS:C	2.36	0.46
2:O:227:ARG:O	2:O:228:SER:O	2.33	0.46
2:O:385:GLU:HB3	2:O:391:THR:O	2.15	0.46
5:E:141:HIS:HB3	19:E:501:FES:S2	2.55	0.46
3:C:121:LEU:O	3:C:125:MET:HG3	2.16	0.46
2:B:307:PHE:CD1	2:B:308:ASP:N	2.83	0.46
3:P:13:LYS:O	3:P:17:ASN:HB2	2.15	0.46
2:O:239:TYR:CD2	2:O:239:TYR:C	2.89	0.46
10:W:52:TRP:O	10:W:56:LYS:HB2	2.15	0.46
1:N:344:ARG:HG3	1:N:344:ARG:NH1	2.26	0.46
2:O:325:TYR:C	2:O:325:TYR:CD2	2.89	0.46
2:B:29:LEU:HB3	2:B:30:PRO:CD	2.45	0.46
5:E:62:LEU:HD12	3:P:164:TRP:CZ2	2.51	0.46
4:Q:167:GLU:HG3	8:U:13:LEU:HD12	1.97	0.46
4:Q:32:VAL:HG11	4:Q:186:VAL:HB	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:ALA:HB1	1:A:428:ILE:HG21	1.98	0.46
3:C:313:GLN:NE2	6:F:36:THR:OG1	2.38	0.46
3:P:123:THR:CG2	3:P:190:ILE:HG13	2.46	0.46
3:P:364:LEU:O	3:P:368:PRO:HG3	2.15	0.46
4:D:148:HIS:ND1	4:D:161:ALA:HA	2.30	0.46
1:N:269:VAL:HG21	1:N:410:VAL:HG21	1.98	0.46
1:A:114:ALA:HB2	1:A:216:PHE:CE2	2.50	0.46
1:N:281:ASP:OD2	1:N:284:PHE:HE1	1.99	0.46
6:F:100:GLU:O	6:F:104:ARG:HG3	2.16	0.46
2:O:132:PHE:CE1	2:O:191:LEU:HB3	2.50	0.46
8:H:15:ASP:O	8:H:17:LEU:N	2.49	0.46
1:A:192:ALA:N	1:A:193:PRO:HD2	2.30	0.46
6:S:51:PRO:HD2	6:S:54:LEU:HD12	1.98	0.46
4:Q:186:VAL:O	4:Q:189:PHE:HB3	2.14	0.46
5:R:58:PHE:O	5:R:61:SER:HB3	2.15	0.46
5:R:120:PRO:O	5:R:121:GLN:CG	2.62	0.46
2:O:168:TYR:CD2	2:O:172:LEU:HB2	2.51	0.46
5:R:100:HIS:HB2	5:R:132:TRP:CZ3	2.51	0.46
5:R:77:LYS:HE2	5:R:79:SER:HB2	1.98	0.46
3:C:90:PHE:CE1	3:C:236:MET:HB3	2.51	0.46
2:B:402:ILE:HD13	2:B:402:ILE:O	2.16	0.46
5:E:109:GLU:OE2	5:E:153:PHE:HB3	2.15	0.46
1:A:146:THR:O	1:A:150:PHE:HD1	1.99	0.46
4:D:150:ASN:O	4:D:156:GLN:HA	2.15	0.46
2:B:385:GLU:HB3	2:B:391:THR:O	2.16	0.46
6:F:59:MET:HA	6:F:59:MET:CE	2.46	0.46
5:R:163:SER:OG	5:R:176:ALA:HB2	2.16	0.46
2:O:206:LEU:CD2	2:O:220:ALA:HB2	2.42	0.46
2:B:325:TYR:CD2	2:B:325:TYR:C	2.88	0.46
1:N:390:ILE:HG23	1:N:394:GLU:CD	2.36	0.46
2:B:290:SER:C	2:B:297:GLN:HE21	2.19	0.46
3:P:123:THR:HG21	3:P:190:ILE:HG13	1.97	0.46
1:N:264:ASP:HA	1:N:265:PRO:HD3	1.75	0.46
5:E:188:VAL:HG12	5:E:188:VAL:O	2.16	0.46
2:B:206:LEU:HG	2:B:206:LEU:O	2.16	0.46
2:O:144:LEU:HB2	2:O:183:ILE:HD12	1.98	0.46
2:B:67:HIS:O	2:B:70:ARG:HB3	2.15	0.46
3:P:338:TRP:NE1	7:T:59:TYR:CE1	2.83	0.46
5:E:90:LYS:HE3	5:E:93:GLY:HA2	1.98	0.46
2:B:368:TYR:O	2:B:371:SER:HB2	2.16	0.46
5:E:45:VAL:CG1	10:J:28:ALA:HA	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:118:ARG:O	5:R:120:PRO:CD	2.56	0.46
9:V:63:ASP:O	9:V:64:LEU:HB2	2.16	0.46
1:N:106:MET:CE	1:N:110:VAL:CG2	2.94	0.46
4:D:70:VAL:HG21	4:D:83:ARG:NH2	2.30	0.46
1:N:145:MET:CB	1:N:252:HIS:CD2	2.99	0.46
2:B:414:ALA:O	2:B:418:VAL:HG23	2.16	0.46
2:O:124:LEU:O	2:O:128:THR:HG23	2.16	0.46
3:C:134:LEU:HD21	3:C:180:PHE:HA	1.98	0.46
5:E:74:ILE:HG22	5:E:91:TRP:CD1	2.51	0.46
2:O:252:LEU:HD11	9:V:49:LEU:HB2	1.97	0.45
2:B:170:THR:O	2:B:172:LEU:N	2.49	0.45
3:P:271:PRO:HB2	3:P:275:PHE:HB2	1.97	0.45
3:C:22:LEU:CD2	13:C:2002:UQ:HM32	2.43	0.45
2:O:181:TYR:CZ	2:O:182:ARG:HG3	2.51	0.45
1:N:191:LYS:O	1:N:195:MET:HG3	2.16	0.45
3:C:13:LYS:O	3:C:17:ASN:HB2	2.16	0.45
3:P:92:PHE:O	3:P:95:ILE:HG22	2.16	0.45
1:A:351:GLU:O	1:A:354:VAL:HG22	2.16	0.45
4:Q:99:GLU:H	4:Q:99:GLU:CD	2.19	0.45
1:N:156:THR:HA	5:R:7:VAL:HG21	1.96	0.45
6:S:67:ASP:HA	6:S:70:LEU:HD23	1.99	0.45
5:R:171:ILE:HG21	5:R:177:PRO:O	2.16	0.45
5:R:109:GLU:OE2	5:R:168:SER:HB2	2.17	0.45
1:N:416:TYR:OH	1:N:442:TYR:HB2	2.16	0.45
2:B:153:GLN:NE2	9:I:34:UNK:CG	2.79	0.45
5:R:116:LYS:O	5:R:117:LEU:HD23	2.16	0.45
2:B:307:PHE:H	9:I:52:ARG:HG2	1.80	0.45
3:C:98:HIS:CD2	11:C:502:HEM:NC	2.83	0.45
5:R:100:HIS:HA	5:R:131:GLU:O	2.16	0.45
5:R:77:LYS:HE3	5:R:191:ASP:OD2	2.16	0.45
2:O:200:THR:OG1	2:O:203:ARG:HD3	2.16	0.45
3:P:6:ARG:O	3:P:13:LYS:HA	2.16	0.45
3:C:6:ARG:HG2	3:C:16:ASN:CB	2.46	0.45
5:E:99:ARG:HB3	5:E:133:VAL:CG1	2.46	0.45
1:N:281:ASP:OD1	1:N:281:ASP:C	2.55	0.45
3:P:151:PHE:HB2	3:P:162:VAL:CG2	2.46	0.45
4:D:117:VAL:O	4:D:123:GLY:HA2	2.16	0.45
3:C:231:LEU:O	3:C:235:LEU:HG	2.16	0.45
1:N:79:VAL:O	1:N:82:MET:HG2	2.16	0.45
1:N:64:PHE:HE2	1:N:86:PHE:CZ	2.34	0.45
2:O:157:VAL:HG22	2:O:157:VAL:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:16:ASN:OD1	3:C:21:ASP:OD1	2.34	0.45
1:A:106:MET:HG3	1:A:203:ILE:CD1	2.45	0.45
2:B:189:GLU:O	2:B:190:GLN:C	2.54	0.45
2:B:71:LEU:HD22	9:I:68:ILE:HG13	1.98	0.45
6:S:100:GLU:O	6:S:104:ARG:HG3	2.17	0.45
9:I:38:UNK:C	9:I:40:UNK:N	2.76	0.45
3:P:166:TRP:HA	3:P:175:THR:HG23	1.99	0.45
3:C:82:ASN:HD22	3:C:82:ASN:N	2.14	0.45
3:P:327:TRP:CE2	7:T:48:VAL:HG22	2.52	0.45
9:I:33:UNK:O	9:I:34:UNK:O	2.34	0.45
2:O:172:LEU:HD13	2:O:316:TYR:CD1	2.51	0.45
2:B:96:LEU:HD12	2:B:97:SER:N	2.32	0.45
7:T:72:LYS:HE2	8:U:57:GLU:OE1	2.15	0.45
5:R:161:HIS:HB2	19:R:501:FES:S1	2.57	0.45
2:O:29:LEU:HB3	2:O:30:PRO:HD2	1.98	0.45
1:A:351:GLU:HA	1:A:354:VAL:HG22	1.99	0.45
1:N:236:PHE:HB2	1:N:258:GLU:OE1	2.17	0.45
3:P:344:VAL:O	3:P:345:GLU:HG3	2.16	0.45
4:D:14:HIS:HB3	4:D:21:LEU:HA	1.99	0.45
1:N:112:LEU:O	1:N:113:LEU:C	2.55	0.45
10:W:10:TYR:HE2	10:W:15:ARG:HD2	1.81	0.45
4:Q:167:GLU:CG	8:U:13:LEU:HD12	2.47	0.45
8:U:65:ARG:O	8:U:69:VAL:HG23	2.17	0.45
6:F:73:ARG:HD3	6:F:73:ARG:HA	1.85	0.45
5:E:171:ILE:HG21	5:E:177:PRO:O	2.16	0.45
4:Q:47:ALA:N	4:Q:50:ASN:HD22	2.02	0.45
1:N:90:THR:O	1:N:167:VAL:HG11	2.15	0.45
9:I:71:ASN:N	9:I:71:ASN:HD22	2.09	0.45
10:J:7:ARG:NH1	10:J:7:ARG:HB3	2.30	0.45
1:N:231:LEU:CD2	1:N:232:PRO:HD2	2.44	0.45
2:O:31:ASN:H	2:O:31:ASN:HD22	1.62	0.45
4:D:99:GLU:H	4:D:99:GLU:CD	2.20	0.45
1:N:354:VAL:HG11	1:N:404:ALA:HA	1.99	0.45
10:J:58:LYS:HB2	10:J:59:TYR:CE1	2.52	0.45
2:O:70:ARG:HG3	2:O:98:VAL:CG1	2.47	0.45
4:Q:97:ASN:HB2	4:Q:98:PRO:HD2	1.99	0.45
1:A:274:ASN:ND2	1:A:309:THR:HB	2.32	0.45
1:N:131:ARG:NH2	1:N:177:LEU:O	2.50	0.45
5:R:112:VAL:HG11	5:R:170:ARG:CZ	2.47	0.45
1:N:106:MET:CE	1:N:110:VAL:HG21	2.47	0.45
2:B:424:MET:HG2	2:B:425:ALA:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:89:SER:O	3:P:90:PHE:C	2.55	0.45
3:P:338:TRP:NE1	7:T:59:TYR:HE1	2.15	0.45
1:N:30:SER:O	1:N:202:GLY:HA2	2.15	0.45
2:O:294:LYS:NZ	2:O:356:ASP:OD2	2.41	0.45
3:C:147:ILE:HG13	12:C:2001:IKR:H16A	1.99	0.45
5:R:102:THR:O	5:R:106:ILE:HG13	2.16	0.45
1:A:269:VAL:HG21	1:A:410:VAL:HG21	1.98	0.45
2:O:307:PHE:CD1	2:O:308:ASP:N	2.85	0.45
7:G:68:ARG:NH2	7:G:69:LEU:HD21	2.31	0.45
3:P:207:ASN:ND2	3:P:208:ASN:H	2.15	0.45
3:P:101:ARG:HD2	3:P:102:GLY:N	2.32	0.45
1:A:106:MET:CG	1:A:203:ILE:HD13	2.46	0.45
1:N:147:ASN:O	1:N:149:THR:N	2.50	0.45
1:A:251:ALA:HB2	1:A:427:PRO:HG2	1.99	0.45
1:N:19:LEU:O	1:N:21:ASN:N	2.50	0.45
5:E:191:ASP:N	5:E:191:ASP:OD2	2.49	0.45
2:O:353:THR:HB	2:O:356:ASP:CG	2.38	0.45
2:B:146:VAL:O	2:B:149:ALA:N	2.50	0.45
5:E:78:LEU:HD11	5:E:187:PHE:HE2	1.80	0.45
2:O:325:TYR:HD2	2:O:325:TYR:C	2.20	0.45
1:A:249:PRO:HG2	1:A:250:VAL:N	2.29	0.45
3:C:92:PHE:HA	3:C:95:ILE:HG22	1.99	0.45
2:B:168:TYR:CD2	2:B:172:LEU:HB2	2.52	0.44
2:O:168:TYR:HE2	2:O:172:LEU:HD12	1.82	0.44
13:C:2002:UQ:HM51	13:C:2002:UQ:H8	1.99	0.44
7:T:36:ASN:O	7:T:40:ARG:HG3	2.15	0.44
1:N:282:ARG:NH2	9:V:37:UNK:N	2.65	0.44
2:B:325:TYR:HD2	2:B:325:TYR:C	2.21	0.44
4:Q:54:VAL:HG11	4:Q:192:TRP:HE1	1.82	0.44
4:D:91:PHE:HA	4:D:92:PRO:HD3	1.76	0.44
4:D:149:TYR:CE1	4:D:156:GLN:HB3	2.52	0.44
3:P:261:ASN:ND2	3:P:264:VAL:HG23	2.32	0.44
2:O:86:THR:O	2:O:90:GLU:HG3	2.17	0.44
3:P:109:LEU:HA	3:P:109:LEU:HD23	1.77	0.44
3:C:75:GLN:OE1	3:C:75:GLN:HA	2.17	0.44
2:B:150:VAL:HG23	2:B:151:ALA:N	2.32	0.44
2:O:25:GLU:HB2	2:O:213:HIS:ND1	2.32	0.44
5:R:109:GLU:CG	5:R:123:ASP:HB2	2.47	0.44
4:D:147:LEU:C	4:D:148:HIS:HD2	2.21	0.44
2:O:26:ILE:HA	2:O:35:ILE:O	2.17	0.44
5:E:86:ASN:ND2	5:E:148:ALA:HB2	2.27	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:P:3002:UQ:HM51	13:P:3002:UQ:H8	1.98	0.44
2:B:27:THR:HG22	2:B:28:LYS:N	2.32	0.44
3:P:278:ALA:HB1	3:P:295:LEU:HD13	1.98	0.44
3:C:158:GLY:O	3:C:160:THR:N	2.50	0.44
4:Q:46:VAL:HB	4:Q:91:PHE:CE2	2.53	0.44
5:E:75:GLU:HG3	5:E:75:GLU:O	2.17	0.44
1:N:134:ILE:HG21	1:N:174:ILE:CG1	2.47	0.44
1:N:58:PHE:HA	1:N:134:ILE:HD11	1.98	0.44
2:O:286:LYS:HE2	2:O:287:ARG:NH2	2.33	0.44
4:D:24:SER:OG	10:J:55:ILE:HG21	2.17	0.44
2:B:133:ARG:HD3	2:B:135:TRP:CZ2	2.52	0.44
4:Q:14:HIS:HB3	4:Q:21:LEU:HA	2.00	0.44
5:E:175:PRO:O	5:E:176:ALA:C	2.55	0.44
1:N:82:MET:CE	1:N:105:ASP:HB3	2.48	0.44
9:V:64:LEU:CD1	9:V:77:ARG:C	2.85	0.44
2:B:43:PRO:O	2:B:113:ARG:HG3	2.17	0.44
1:A:106:MET:CE	1:A:110:VAL:CG2	2.95	0.44
2:O:31:ASN:H	2:O:31:ASN:ND2	2.15	0.44
2:B:72:ALA:HB1	2:B:75:LEU:HD12	2.00	0.44
2:O:374:THR:HG22	2:O:376:GLN:HB3	1.99	0.44
3:P:151:PHE:C	3:P:153:ALA:H	2.21	0.44
2:B:105:MET:HE2	2:B:107:TYR:CE1	2.53	0.44
3:P:319:ARG:HB3	3:P:374:GLU:OE1	2.17	0.44
3:P:175:THR:O	3:P:178:ARG:HG2	2.17	0.44
2:B:268:GLU:HG2	2:B:272:PHE:HE1	1.81	0.44
5:R:79:SER:OG	5:R:191:ASP:CB	2.65	0.44
2:O:72:ALA:HB1	2:O:75:LEU:HD12	1.98	0.44
4:Q:171:TYR:OH	4:Q:182:ILE:HA	2.17	0.44
3:P:234:THR:HG21	4:Q:219:LEU:HD12	1.99	0.44
1:N:147:ASN:C	1:N:149:THR:N	2.68	0.44
1:N:19:LEU:C	1:N:21:ASN:H	2.21	0.44
4:D:164:ILE:O	4:D:179:MET:CE	2.65	0.44
1:A:45:SER:OG	1:A:92:ARG:HA	2.18	0.44
1:A:269:VAL:HG22	1:A:406:MET:HE2	1.98	0.44
10:W:60:GLU:O	10:W:61:ALA:CB	2.65	0.44
17:D:501:HEC:HHA	17:D:501:HEC:HBA1	2.00	0.44
3:C:278:ALA:HB1	3:C:295:LEU:HD13	1.99	0.44
6:S:12:LEU:C	6:S:14:ASP:N	2.71	0.44
5:R:53:ASN:O	5:R:57:GLN:HG3	2.17	0.44
1:A:390:ILE:HG23	1:A:394:GLU:CD	2.38	0.44
4:Q:14:HIS:CG	4:Q:21:LEU:HD23	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:17:PRO:O	4:D:202:LYS:HD3	2.17	0.44
1:A:264:ASP:HA	1:A:265:PRO:HD3	1.75	0.44
3:P:279:TYR:O	3:P:282:LEU:HB3	2.18	0.44
1:N:192:ALA:N	1:N:193:PRO:HD2	2.32	0.44
4:D:43:MET:HG3	4:D:46:VAL:HG23	1.99	0.44
4:D:43:MET:HE3	4:D:91:PHE:HE2	1.82	0.44
8:H:21:ARG:HG3	8:H:21:ARG:NH1	2.33	0.44
1:A:223:TYR:OH	1:A:224:LYS:HE3	2.17	0.44
3:P:33:ASN:HB3	20:P:386:HOH:O	2.16	0.44
1:A:177:LEU:HD22	1:A:181:ASP:HB2	2.00	0.44
4:D:2:GLU:CB	7:G:70:LYS:HE2	2.39	0.44
3:P:342:GLN:HB3	3:P:348:PHE:CE1	2.52	0.44
5:R:113:ASP:O	5:R:115:SER:N	2.51	0.44
6:S:13:MET:O	6:S:17:ARG:HG3	2.18	0.44
5:R:136:VAL:HG23	5:R:183:PRO:HD3	2.00	0.44
4:D:218:LEU:HD13	5:E:43:ALA:N	2.33	0.44
1:A:438:ARG:HG3	1:A:438:ARG:NH1	2.33	0.44
5:E:53:ASN:O	5:E:57:GLN:HG3	2.18	0.44
9:V:39:UNK:O	9:V:40:UNK:C	2.66	0.44
7:G:28:ASN:HB2	7:G:32:ASP:HB3	1.98	0.44
2:O:275:LEU:O	2:O:275:LEU:HD12	2.18	0.44
2:B:80:ALA:HA	2:B:84:ARG:NH1	2.23	0.44
2:B:238:THR:CG2	2:B:239:TYR:N	2.80	0.44
3:P:31:TRP:NE1	15:P:3007:PEE:O4	2.51	0.44
5:E:86:ASN:HD22	5:E:148:ALA:CB	2.27	0.44
8:U:34:ARG:O	8:U:34:ARG:HD3	2.17	0.44
1:N:45:SER:HA	1:N:48:GLU:CD	2.38	0.44
3:P:75:GLN:OE1	3:P:75:GLN:HA	2.18	0.44
3:C:184:PHE:HD2	3:C:184:PHE:O	2.01	0.44
2:B:153:GLN:NE2	9:I:34:UNK:HG2	2.33	0.43
1:N:206:LYS:O	1:N:208:LEU:N	2.51	0.43
4:Q:102:ARG:HA	4:Q:108:ALA:O	2.18	0.43
2:B:46:ARG:HD3	2:B:110:GLU:HG2	1.99	0.43
1:A:197:LEU:HD13	1:A:216:PHE:CE1	2.53	0.43
2:O:306:PRO:HB3	9:V:51:CYS:C	2.39	0.43
1:A:354:VAL:HG11	1:A:404:ALA:HA	1.99	0.43
2:O:59:THR:HG22	2:O:60:THR:N	2.33	0.43
5:R:75:GLU:O	5:R:75:GLU:HG3	2.18	0.43
7:G:46:PHE:O	7:G:50:PRO:HG2	2.18	0.43
3:C:18:SER:HB2	3:C:202:HIS:CE1	2.48	0.43
1:N:135:LEU:CD2	1:N:174:ILE:HG21	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:106:ILE:O	5:E:106:ILE:HG22	2.18	0.43
1:A:35:CYS:SG	1:A:203:ILE:HD11	2.58	0.43
9:I:59:SER:O	9:I:60:ALA:C	2.56	0.43
1:A:64:PHE:HE2	1:A:86:PHE:CZ	2.36	0.43
2:B:350:GLY:H	2:B:411:VAL:HG11	1.82	0.43
5:R:15:ARG:NH1	5:R:32:ARG:HB3	2.33	0.43
3:P:219:ILE:HD12	3:P:224:TYR:CD1	2.53	0.43
2:O:306:PRO:HB3	9:V:51:CYS:HA	1.99	0.43
4:Q:110:PRO:HA	4:Q:111:PRO:HD2	1.92	0.43
4:Q:151:PRO:HA	4:Q:156:GLN:HG3	2.00	0.43
1:A:411:CYS:HB3	1:A:415:ILE:HD12	1.99	0.43
8:U:72:LYS:O	8:U:74:PHE:N	2.51	0.43
9:I:28:UNK:N	9:I:72:ALA:HB2	2.33	0.43
4:Q:231:LYS:HD3	6:S:71:LYS:HA	2.00	0.43
2:O:168:TYR:HB2	2:O:173:ALA:CB	2.43	0.43
3:C:364:LEU:O	3:C:368:PRO:HG3	2.19	0.43
3:C:6:ARG:O	3:C:13:LYS:HA	2.19	0.43
2:B:338:ARG:O	2:B:341:MET:HB2	2.18	0.43
4:Q:70:VAL:HG21	4:Q:83:ARG:NH2	2.33	0.43
3:P:34:PHE:CD1	3:P:37:LEU:HD12	2.54	0.43
1:N:281:ASP:CB	9:V:33:UNK:HB2	2.49	0.43
4:D:16:GLY:N	4:D:19:SER:OG	2.50	0.43
2:O:225:ASN:O	2:O:227:ARG:CG	2.65	0.43
4:D:238:ARG:CZ	5:E:5:VAL:HG22	2.49	0.43
4:Q:178:THR:HG21	8:U:16:PRO:HD2	2.01	0.43
5:E:142:LEU:HD12	5:E:161:HIS:CE1	2.53	0.43
9:V:49:LEU:O	9:V:50:LEU:HD23	2.19	0.43
9:I:33:UNK:HG2	9:I:73:PRO:HB3	2.00	0.43
2:B:167:ALA:C	2:B:168:TYR:CD1	2.92	0.43
5:E:100:HIS:CD2	5:E:131:GLU:HB2	2.53	0.43
2:O:164:HIS:O	2:O:173:ALA:HA	2.19	0.43
1:N:269:VAL:HG11	1:N:410:VAL:HG21	1.99	0.43
2:O:365:LYS:O	2:O:369:LEU:HG	2.17	0.43
4:D:181:GLN:CA	8:H:77:LEU:HD22	2.48	0.43
2:O:399:ALA:HA	2:O:402:ILE:HG22	1.99	0.43
5:R:69:LEU:O	5:R:72:SER:CB	2.67	0.43
3:P:261:ASN:ND2	3:P:264:VAL:CG2	2.81	0.43
2:B:435:PHE:O	2:B:438:GLU:N	2.52	0.43
1:N:429:GLU:OE2	7:T:7:LEU:HB2	2.18	0.43
5:E:119:ASP:O	5:E:121:GLN:N	2.52	0.43
5:E:141:HIS:HB2	5:E:176:ALA:CA	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:353:THR:HB	2:B:356:ASP:OD1	2.18	0.43
1:A:87:ASN:OD1	2:B:286:LYS:HD2	2.18	0.43
1:N:23:LEU:HD23	1:N:24:ARG:N	2.33	0.43
1:A:79:VAL:O	1:A:82:MET:HG2	2.18	0.43
3:C:219:ILE:HB	3:C:224:TYR:HD1	1.82	0.43
3:C:41:CYS:SG	3:C:91:PHE:HA	2.58	0.43
1:A:244:ARG:CZ	7:G:10:VAL:HB	2.48	0.43
1:A:239:SER:HB2	7:G:17:SER:O	2.18	0.43
1:N:159:GLN:NE2	1:N:237:THR:HG21	2.33	0.43
3:C:133:VAL:HG22	3:C:144:ALA:HB2	2.01	0.43
2:O:312:PHE:O	2:O:322:PHE:HA	2.18	0.43
1:A:131:ARG:NH2	1:A:177:LEU:O	2.52	0.43
9:I:33:UNK:HG3	9:I:73:PRO:HB3	2.01	0.43
2:O:309:ALA:HA	2:O:325:TYR:O	2.18	0.43
5:R:148:ALA:O	5:R:149:ASN:CB	2.66	0.43
5:R:99:ARG:HB3	5:R:133:VAL:CG1	2.47	0.43
2:B:28:LYS:HG2	2:B:28:LYS:O	2.18	0.43
2:O:306:PRO:HB3	9:V:51:CYS:CA	2.49	0.43
2:B:70:ARG:HG3	2:B:98:VAL:HG12	1.99	0.43
4:D:162:PRO:HA	4:D:163:PRO:HD2	1.89	0.43
1:N:236:PHE:CB	1:N:258:GLU:OE1	2.66	0.43
4:D:27:ARG:O	4:D:30:PHE:HB3	2.18	0.43
4:Q:76:GLU:CD	4:Q:76:GLU:H	2.21	0.43
8:H:43:ARG:HG3	8:H:44:VAL:N	2.33	0.43
1:N:50:GLU:O	1:N:50:GLU:HG2	2.18	0.43
1:A:103:SER:O	1:A:106:MET:HB2	2.18	0.43
4:Q:237:TYR:HB2	6:S:60:PHE:CD2	2.52	0.43
3:P:64:PHE:CE1	16:P:3011:GOL:H12	2.53	0.43
2:B:385:GLU:O	2:B:387:LEU:N	2.51	0.43
5:R:20:ASP:C	5:R:22:THR:H	2.22	0.43
3:C:36:SER:O	3:C:40:VAL:HG23	2.18	0.43
1:A:241:ILE:HG23	1:A:241:ILE:O	2.19	0.43
1:A:163:LEU:HD23	1:A:163:LEU:HA	1.83	0.43
5:E:59:ILE:HA	5:E:59:ILE:HD13	1.82	0.43
2:O:76:THR:HG23	2:O:82:SER:HB2	2.00	0.43
5:R:135:LEU:HD13	5:R:180:LEU:HD12	2.00	0.43
4:Q:222:MET:HE3	5:R:40:THR:CG2	2.43	0.43
7:G:80:ASP:O	7:G:81:GLN:C	2.57	0.43
2:O:109:VAL:CG2	2:O:119:VAL:HG12	2.47	0.43
3:C:245:LEU:HD23	3:C:245:LEU:HA	1.84	0.43
3:C:151:PHE:C	3:C:153:ALA:H	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:ASN:O	1:A:149:THR:N	2.52	0.43
3:C:156:TYR:C	3:C:158:GLY:H	2.22	0.43
6:F:16:ILE:O	6:F:19:TRP:HB3	2.19	0.43
1:A:6:GLN:C	1:A:8:LEU:N	2.72	0.43
6:F:77:LYS:HA	6:F:80:TRP:CE2	2.54	0.43
4:Q:27:ARG:O	4:Q:30:PHE:HB3	2.18	0.43
5:R:153:PHE:CE2	5:R:172:ARG:NE	2.87	0.43
3:C:19:LEU:O	3:C:20:ILE:HG13	2.18	0.43
2:B:255:ALA:O	2:B:325:TYR:HA	2.19	0.43
1:N:49:ASN:CG	1:N:51:LYS:H	2.22	0.43
5:R:148:ALA:HB2	5:R:156:TYR:CE2	2.53	0.43
5:R:38:LEU:HA	10:W:14:PHE:CE1	2.54	0.43
9:V:28:UNK:CB	9:V:72:ALA:HB2	2.49	0.43
4:Q:43:MET:HE1	4:Q:189:PHE:CZ	2.53	0.43
5:R:1:VAL:CG2	5:R:3:ASN:HD22	2.31	0.43
2:B:209:ILE:HG22	2:B:210:GLY:N	2.33	0.43
8:U:28:GLU:CG	8:U:32:LYS:HE3	2.49	0.43
3:C:367:PHE:N	3:C:368:PRO:HD2	2.34	0.43
2:B:166:ALA:HB1	2:B:242:GLY:C	2.39	0.43
2:B:325:TYR:CD1	9:I:60:ALA:CB	3.02	0.43
3:P:43:MET:HE1	13:P:3002:UQ:C12	2.49	0.43
5:R:29:SER:CA	5:R:32:ARG:HH21	2.32	0.43
3:C:175:THR:O	3:C:178:ARG:HG2	2.18	0.43
1:N:411:CYS:HB3	1:N:415:ILE:HD12	2.01	0.43
2:O:258:VAL:HG21	2:O:321:LEU:HD22	2.01	0.43
2:B:355:GLU:O	2:B:358:THR:HB	2.19	0.42
5:E:75:GLU:HA	5:E:193:VAL:O	2.18	0.42
5:E:164:HIS:CD2	5:E:173:LYS:HB3	2.41	0.42
2:B:26:ILE:HA	2:B:35:ILE:O	2.18	0.42
2:B:374:THR:HG22	2:B:376:GLN:HB3	2.01	0.42
5:R:38:LEU:HB2	10:W:14:PHE:HE1	1.84	0.42
5:E:156:TYR:N	5:E:156:TYR:CD1	2.87	0.42
1:N:45:SER:OG	1:N:92:ARG:HA	2.19	0.42
4:Q:167:GLU:C	4:Q:169:LEU:N	2.71	0.42
3:C:37:LEU:O	3:C:41:CYS:HB2	2.18	0.42
3:P:133:VAL:HA	3:P:140:SER:HB3	2.01	0.42
6:S:42:ASP:OD1	6:S:101:ARG:NH1	2.52	0.42
2:B:59:THR:HG22	2:B:60:THR:N	2.33	0.42
3:P:266:PRO:HA	3:P:267:PRO:HD3	1.84	0.42
3:P:82:ASN:HD22	3:P:82:ASN:N	2.15	0.42
8:U:43:ARG:HG3	8:U:44:VAL:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:51:ILE:HG22	2:B:52:LYS:N	2.35	0.42
5:E:100:HIS:HD2	5:E:131:GLU:HB2	1.84	0.42
3:P:6:ARG:HD3	3:P:16:ASN:OD1	2.19	0.42
3:C:19:LEU:C	3:C:20:ILE:HG13	2.39	0.42
2:O:350:GLY:H	2:O:411:VAL:HG11	1.84	0.42
1:A:341:GLU:HA	1:A:344:ARG:HB2	2.01	0.42
4:Q:143:VAL:HG21	4:Q:149:TYR:HB2	2.01	0.42
2:O:353:THR:HG22	2:O:354:GLU:N	2.34	0.42
3:P:325:LEU:HD22	3:P:370:ILE:HG13	2.01	0.42
2:O:150:VAL:HG23	2:O:151:ALA:N	2.34	0.42
2:B:424:MET:HB2	2:B:436:LEU:HD13	2.01	0.42
3:P:379:ASN:HA	6:S:17:ARG:HH12	1.85	0.42
4:Q:66:GLU:C	4:Q:68:VAL:H	2.23	0.42
2:B:246:GLU:HG2	2:B:246:GLU:O	2.19	0.42
1:N:130:GLU:O	1:N:134:ILE:HG13	2.19	0.42
1:N:135:LEU:HD23	1:N:135:LEU:HA	1.86	0.42
2:O:325:TYR:HB3	9:V:59:SER:HB3	2.01	0.42
3:P:172:ASP:OD1	3:P:173:ASN:N	2.40	0.42
7:T:77:TYR:C	7:T:79:ASN:N	2.72	0.42
1:A:153:LEU:O	1:A:156:THR:HG22	2.18	0.42
11:P:502:HEM:HMB1	11:P:502:HEM:HBB2	2.00	0.42
1:N:281:ASP:O	1:N:283:THR:N	2.52	0.42
1:N:44:GLY:HA3	1:N:92:ARG:O	2.19	0.42
4:Q:169:LEU:HG	4:Q:170:GLU:N	2.34	0.42
3:P:365:ILE:HG22	3:P:366:LEU:N	2.35	0.42
1:A:90:THR:HB	1:A:95:THR:HG23	2.01	0.42
5:R:186:GLN:NE2	5:R:188:VAL:HG13	2.33	0.42
5:R:83:GLU:HA	5:R:100:HIS:O	2.19	0.42
8:U:15:ASP:C	8:U:17:LEU:N	2.73	0.42
8:U:15:ASP:O	8:U:17:LEU:N	2.52	0.42
5:E:147:ILE:HD11	5:E:159:PRO:HG3	2.01	0.42
7:G:30:PHE:O	7:G:35:PRO:CD	2.68	0.42
5:E:20:ASP:C	5:E:22:THR:H	2.23	0.42
9:I:41:UNK:O	9:I:42:UNK:C	2.67	0.42
1:A:315:SER:OG	1:A:316:ASP:N	2.52	0.42
2:O:344:LEU:HD13	2:O:417:PHE:CE2	2.55	0.42
5:R:39:VAL:O	5:R:42:THR:HB	2.20	0.42
2:B:124:LEU:C	2:B:124:LEU:HD23	2.39	0.42
3:P:224:TYR:HB3	4:Q:227:TRP:CZ2	2.54	0.42
2:O:46:ARG:HD3	2:O:110:GLU:HG2	2.02	0.42
4:Q:164:ILE:HG21	4:Q:182:ILE:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:80:TRP:CD1	6:S:80:TRP:N	2.86	0.42
4:Q:149:TYR:CE1	4:Q:156:GLN:HB3	2.55	0.42
1:N:313:SER:O	1:N:314:TYR:CD2	2.72	0.42
3:C:284:SER:O	3:C:286:PRO:HD3	2.18	0.42
2:B:193:HIS:O	2:B:197:ASN:ND2	2.53	0.42
5:E:10:PHE:CD1	7:G:18:LEU:HD21	2.54	0.42
4:D:167:GLU:C	4:D:169:LEU:N	2.73	0.42
1:A:310:PHE:CD2	1:A:310:PHE:C	2.93	0.42
1:N:383:LEU:HD23	1:N:388:ARG:HA	2.02	0.42
1:A:171:THR:O	1:A:175:LYS:HG3	2.20	0.42
1:N:24:ARG:NH2	1:N:193:PRO:O	2.53	0.42
2:B:189:GLU:O	2:B:191:LEU:N	2.53	0.42
2:O:280:GLY:HA3	2:O:293:SER:OG	2.20	0.42
3:P:346:HIS:CG	3:P:347:PRO:HA	2.54	0.42
2:B:141:GLN:N	2:B:142:PRO:HD2	2.33	0.42
4:Q:16:GLY:HA3	4:Q:19:SER:OG	2.19	0.42
4:Q:16:GLY:N	4:Q:19:SER:OG	2.53	0.42
3:P:287:ASN:O	3:P:289:LEU:N	2.53	0.42
6:S:31:LEU:HD21	6:S:65:ALA:HB2	2.01	0.42
4:D:76:GLU:O	4:Q:99:GLU:HB3	2.20	0.42
8:U:65:ARG:O	8:U:68:CYS:HB3	2.19	0.42
4:Q:14:HIS:CB	4:Q:21:LEU:HD23	2.50	0.42
6:F:13:MET:HE1	6:F:16:ILE:HD12	2.01	0.42
3:C:123:THR:CG2	3:C:190:ILE:HG13	2.49	0.42
10:W:4:ALA:O	10:W:8:GLN:HG3	2.19	0.42
2:O:22:GLU:HG3	2:O:23:ASP:H	1.84	0.42
3:C:30:ALA:C	3:C:32:TRP:H	2.22	0.42
3:C:327:TRP:CE2	7:G:48:VAL:HG22	2.54	0.42
1:N:136:GLN:OE1	9:V:50:LEU:HD13	2.20	0.42
5:R:157:TYR:HD1	5:R:164:HIS:HD1	1.68	0.42
10:W:59:TYR:N	10:W:59:TYR:CD1	2.87	0.42
1:A:206:LYS:O	1:A:207:GLU:C	2.57	0.42
5:E:136:VAL:CG2	5:E:183:PRO:HD3	2.47	0.42
1:A:365:MET:HG3	1:A:366:VAL:N	2.33	0.42
1:A:197:LEU:HD22	1:A:216:PHE:CE1	2.52	0.42
2:O:146:VAL:O	2:O:149:ALA:N	2.53	0.42
2:O:355:GLU:O	2:O:358:THR:HB	2.20	0.42
2:O:167:ALA:C	2:O:168:TYR:CD1	2.93	0.42
1:N:191:LYS:CA	1:N:195:MET:HE2	2.50	0.42
2:B:220:ALA:O	2:B:224:LEU:HB2	2.20	0.42
8:H:34:ARG:O	8:H:38:GLU:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:179:MET:O	4:Q:182:ILE:HB	2.19	0.42
1:A:24:ARG:NH2	1:A:193:PRO:O	2.53	0.42
2:O:124:LEU:HD23	2:O:124:LEU:C	2.39	0.42
1:N:298:ALA:HA	1:N:303:LEU:HD12	2.02	0.42
1:N:6:GLN:C	1:N:8:LEU:N	2.73	0.42
4:D:32:VAL:HG11	4:D:186:VAL:HB	2.01	0.42
7:G:41:PHE:CE2	7:G:45:VAL:HG21	2.55	0.42
5:R:102:THR:OG1	5:R:105:GLU:HG3	2.20	0.42
5:R:78:LEU:N	5:R:191:ASP:O	2.53	0.42
3:C:297:ALA:O	3:C:301:ILE:HB	2.20	0.42
1:A:106:MET:CE	1:A:110:VAL:HG21	2.49	0.42
2:O:215:ASP:O	2:O:219:VAL:HG23	2.19	0.42
1:N:279:ARG:HA	1:N:307:PHE:CE1	2.55	0.42
1:N:156:THR:HG23	1:N:157:ALA:N	2.35	0.42
3:P:165:ALA:O	3:P:178:ARG:HD2	2.19	0.42
1:A:310:PHE:CD2	1:A:310:PHE:O	2.73	0.42
3:C:61:SER:O	3:C:62:LEU:HD23	2.20	0.42
4:D:234:LYS:HD2	5:E:8:PRO:HB2	2.01	0.42
3:C:276:LEU:HB2	3:C:337:THR:HG23	2.02	0.42
3:C:38:LEU:HD23	3:C:38:LEU:HA	1.83	0.42
5:R:78:LEU:HD22	5:R:132:TRP:CE2	2.55	0.41
2:O:239:TYR:C	2:O:239:TYR:HD2	2.23	0.41
7:G:80:ASP:HB3	8:H:50:THR:CA	2.46	0.41
17:Q:501:HEC:HBA1	17:Q:501:HEC:HHA	2.01	0.41
8:H:15:ASP:C	8:H:17:LEU:N	2.73	0.41
3:C:325:LEU:HD22	3:C:370:ILE:HG13	2.02	0.41
4:D:239:PRO:HA	4:D:240:PRO:HD3	1.95	0.41
3:C:40:VAL:O	3:C:44:THR:OG1	2.38	0.41
5:E:104:ALA:O	5:E:108:GLN:HB3	2.19	0.41
5:E:189:GLY:O	5:E:192:LEU:N	2.53	0.41
1:N:255:LEU:O	1:N:321:GLY:HA3	2.21	0.41
1:A:117:VAL:CG2	1:A:118:GLN:N	2.80	0.41
1:A:156:THR:HG23	1:A:157:ALA:N	2.34	0.41
1:N:261:GLY:HA2	1:N:317:THR:O	2.19	0.41
2:O:277:HIS:NE2	2:O:364:LEU:HD13	2.34	0.41
4:Q:167:GLU:C	4:Q:169:LEU:H	2.22	0.41
4:D:14:HIS:CG	4:D:21:LEU:HD23	2.54	0.41
3:P:305:ILE:HB	3:P:306:PRO:HD3	2.02	0.41
1:N:39:VAL:HG13	1:N:39:VAL:O	2.20	0.41
3:P:365:ILE:O	3:P:368:PRO:HG2	2.20	0.41
5:E:82:PRO:HG2	5:E:85:LYS:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:W:7:ARG:HB3	10:W:7:ARG:NH1	2.36	0.41
2:O:259:THR:O	2:O:260:GLU:C	2.59	0.41
2:B:239:TYR:HE2	2:B:241:GLY:HA2	1.84	0.41
1:N:106:MET:HB3	1:N:107:PRO:HD3	2.02	0.41
1:A:186:ILE:HG13	1:A:186:ILE:H	1.64	0.41
10:J:7:ARG:HH11	10:J:7:ARG:CB	2.34	0.41
1:A:104:LYS:O	1:A:107:PRO:HD2	2.20	0.41
1:A:106:MET:HB3	1:A:107:PRO:HD3	2.01	0.41
3:C:89:SER:O	3:C:90:PHE:C	2.58	0.41
3:C:277:PHE:CG	3:C:278:ALA:N	2.88	0.41
3:C:162:VAL:C	3:C:164:TRP:N	2.74	0.41
3:C:70:THR:HA	3:C:74:VAL:CG2	2.49	0.41
10:J:4:ALA:O	10:J:8:GLN:HG3	2.20	0.41
8:H:65:ARG:O	8:H:68:CYS:HB3	2.21	0.41
7:G:72:LYS:HE2	8:H:57:GLU:OE1	2.19	0.41
2:B:355:GLU:O	2:B:358:THR:N	2.53	0.41
1:N:136:GLN:O	1:N:140:GLU:HG3	2.21	0.41
2:B:372:VAL:HG13	2:B:378:LEU:CA	2.42	0.41
1:A:90:THR:HA	1:A:95:THR:HA	2.02	0.41
2:O:207:VAL:HG21	2:O:383:GLY:CA	2.47	0.41
2:O:238:THR:CG2	2:O:239:TYR:H	2.31	0.41
5:E:30:GLU:HB2	10:J:7:ARG:HG2	2.01	0.41
5:R:156:TYR:CD1	5:R:156:TYR:N	2.87	0.41
2:B:319:SER:OG	2:B:320:GLY:N	2.53	0.41
2:O:291:VAL:C	2:O:293:SER:H	2.24	0.41
1:N:307:PHE:HA	1:N:323:HIS:O	2.20	0.41
4:Q:182:ILE:HG22	4:Q:183:ALA:N	2.35	0.41
3:P:30:ALA:C	3:P:32:TRP:H	2.23	0.41
1:N:153:LEU:O	1:N:156:THR:HG22	2.20	0.41
3:C:336:LEU:HG	3:C:355:ALA:HB1	2.02	0.41
1:N:171:THR:O	1:N:175:LYS:HG3	2.21	0.41
2:B:209:ILE:CG2	2:B:210:GLY:N	2.83	0.41
2:O:338:ARG:O	2:O:341:MET:HB2	2.21	0.41
3:C:120:LEU:HD23	3:C:120:LEU:HA	1.86	0.41
2:B:239:TYR:C	2:B:239:TYR:HD2	2.24	0.41
1:N:106:MET:HB3	1:N:107:PRO:CD	2.50	0.41
1:A:58:PHE:HA	1:A:134:ILE:HD11	2.01	0.41
3:P:90:PHE:CE1	3:P:236:MET:HB3	2.54	0.41
2:O:27:THR:CG2	2:O:28:LYS:H	2.32	0.41
2:B:131:GLU:O	2:B:132:PHE:C	2.57	0.41
2:B:71:LEU:HD11	2:B:144:LEU:HD23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:350:ILE:O	3:P:354:MET:HG2	2.21	0.41
4:D:37:CYS:O	4:D:39:ALA:N	2.52	0.41
3:C:108:TYR:HB3	3:C:114:TRP:CE3	2.55	0.41
1:A:44:GLY:HA3	1:A:92:ARG:O	2.20	0.41
3:P:242:THR:N	4:Q:208:MET:HE1	2.35	0.41
5:R:84:GLY:N	5:R:102:THR:HG23	2.36	0.41
3:P:138:GLN:HG2	3:P:258:THR:HG22	2.03	0.41
2:O:97:SER:HB3	9:V:69:SER:CB	2.51	0.41
1:A:191:LYS:CA	1:A:195:MET:HE2	2.51	0.41
1:A:81:SER:HB3	2:B:359:LYS:HD3	2.02	0.41
3:C:287:ASN:O	3:C:289:LEU:N	2.53	0.41
2:B:278:VAL:O	2:B:294:LYS:HG3	2.20	0.41
3:P:79:LEU:CD2	5:R:57:GLN:NE2	2.84	0.41
3:P:230:ILE:HG21	15:R:3005:PEE:H22	2.02	0.41
1:A:433:ASP:OD2	1:A:435:ASN:HB2	2.20	0.41
3:C:130:VAL:HG23	3:C:131:GLY:N	2.35	0.41
1:A:382:HIS:HB3	1:A:388:ARG:O	2.20	0.41
5:E:129:LYS:HD2	5:E:132:TRP:HD1	1.85	0.41
2:B:238:THR:CG2	2:B:239:TYR:H	2.31	0.41
3:P:105:TYR:CE2	3:P:209:PRO:HA	2.55	0.41
3:C:11:LEU:HA	3:C:14:MET:HG3	2.02	0.41
2:B:37:SER:HB3	2:B:213:HIS:CG	2.55	0.41
2:B:292:THR:HG21	2:B:363:GLN:NE2	2.36	0.41
3:P:162:VAL:C	3:P:164:TRP:N	2.74	0.41
1:N:45:SER:HA	1:N:48:GLU:CG	2.50	0.41
5:E:53:ASN:O	5:E:56:THR:HB	2.19	0.41
4:D:237:TYR:HB2	6:F:60:PHE:CG	2.55	0.41
2:B:168:TYR:HB2	2:B:173:ALA:CB	2.38	0.41
2:O:287:ARG:HG3	2:O:287:ARG:NH1	2.36	0.41
2:B:259:THR:CG2	2:B:260:GLU:N	2.82	0.41
1:N:269:VAL:HG22	1:N:406:MET:CE	2.51	0.41
1:N:145:MET:HB2	1:N:252:HIS:NE2	2.35	0.41
3:P:326:PHE:O	3:P:329:LEU:HB3	2.21	0.41
3:P:151:PHE:C	3:P:153:ALA:N	2.73	0.41
2:O:212:LYS:HG2	2:O:214:SER:OG	2.20	0.41
1:A:358:LYS:HE3	1:A:399:ILE:O	2.21	0.41
2:B:265:GLY:O	2:B:266:SER:C	2.58	0.41
3:C:45:GLN:OE1	3:C:45:GLN:HA	2.20	0.41
1:N:274:ASN:HA	1:N:274:ASN:HD22	1.59	0.41
5:E:119:ASP:HB3	5:E:179:ASN:HD21	1.86	0.41
2:B:164:HIS:O	2:B:173:ALA:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:342:GLN:HA	3:C:342:GLN:NE2	2.35	0.41
5:R:129:LYS:HA	5:R:130:PRO:HD3	1.91	0.41
4:Q:148:HIS:CE1	4:Q:161:ALA:HB2	2.56	0.41
4:Q:161:ALA:O	4:Q:163:PRO:N	2.53	0.41
4:Q:10:PHE:CD1	4:Q:10:PHE:N	2.89	0.41
3:C:173:ASN:N	3:C:174:PRO:CD	2.83	0.41
3:P:120:LEU:HA	3:P:120:LEU:HD23	1.95	0.41
3:C:151:PHE:C	3:C:153:ALA:N	2.74	0.41
2:O:345:LYS:HG2	2:O:418:VAL:CG1	2.51	0.41
1:N:351:GLU:HA	1:N:354:VAL:HG22	2.02	0.41
2:O:141:GLN:N	2:O:142:PRO:HD2	2.36	0.41
6:F:51:PRO:O	6:F:52:GLU:C	2.58	0.41
4:D:46:VAL:HB	4:D:91:PHE:CE2	2.56	0.41
7:G:30:PHE:CD2	7:G:34:LEU:HD12	2.56	0.41
1:A:270:LEU:O	1:A:273:ALA:HB3	2.21	0.41
2:O:133:ARG:HA	2:O:134:PRO:HD3	1.96	0.41
6:F:77:LYS:HB3	6:F:77:LYS:HE2	1.95	0.41
7:G:72:LYS:CE	8:H:57:GLU:OE1	2.69	0.41
4:D:208:MET:O	4:D:212:SER:HB2	2.21	0.41
6:S:59:MET:CE	6:S:59:MET:HA	2.51	0.41
3:P:357:LEU:HA	3:P:357:LEU:HD12	1.92	0.41
3:P:196:ILE:HG22	3:P:200:PHE:CE2	2.56	0.41
4:Q:165:TYR:O	4:Q:166:ASN:C	2.60	0.41
1:A:228:VAL:O	1:A:228:VAL:HG13	2.21	0.41
3:C:109:LEU:HA	3:C:109:LEU:HD23	1.68	0.41
5:R:109:GLU:CD	5:R:123:ASP:HB2	2.41	0.41
1:A:60:GLU:OE2	1:A:89:TYR:HA	2.20	0.41
2:O:206:LEU:O	2:O:206:LEU:HG	2.21	0.41
1:N:104:LYS:O	1:N:107:PRO:HD2	2.21	0.41
1:A:46:ARG:HD3	1:A:231:LEU:HD13	2.03	0.41
2:B:402:ILE:O	2:B:405:VAL:HG23	2.21	0.41
8:H:28:GLU:CG	8:H:32:LYS:HE3	2.50	0.41
2:B:385:GLU:C	2:B:387:LEU:H	2.25	0.41
1:A:45:SER:HA	1:A:48:GLU:HG3	2.02	0.41
2:O:408:ALA:O	2:O:409:ASP:C	2.59	0.41
7:G:53:LEU:O	7:G:57:LEU:HG	2.21	0.41
9:V:49:LEU:HD22	9:V:54:SER:O	2.21	0.40
2:B:181:TYR:CZ	2:B:182:ARG:HG3	2.56	0.40
4:D:148:HIS:CE1	4:D:161:ALA:CB	3.04	0.40
1:N:191:LYS:C	1:N:193:PRO:HD2	2.41	0.40
4:Q:147:LEU:C	4:Q:148:HIS:CD2	2.92	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:MET:HB3	1:A:107:PRO:CD	2.52	0.40
3:C:46:ILE:HA	11:C:501:HEM:HMC2	2.01	0.40
3:P:198:LEU:HA	3:P:198:LEU:HD23	1.90	0.40
5:E:29:SER:CA	5:E:32:ARG:HH21	2.34	0.40
2:O:306:PRO:CB	9:V:51:CYS:HA	2.51	0.40
5:E:157:TYR:O	5:E:159:PRO:HD3	2.21	0.40
4:Q:116:ILE:CG2	4:Q:117:VAL:N	2.84	0.40
2:B:212:LYS:HG2	2:B:214:SER:OG	2.21	0.40
3:C:323:GLN:O	3:C:326:PHE:HB3	2.21	0.40
3:C:344:VAL:O	3:C:345:GLU:HG3	2.22	0.40
1:A:135:LEU:HD23	1:A:135:LEU:HA	1.87	0.40
5:R:166:ASP:OD1	5:R:168:SER:N	2.47	0.40
4:Q:161:ALA:O	4:Q:162:PRO:C	2.59	0.40
3:P:31:TRP:HE1	14:P:3004:CDL:H1	1.86	0.40
3:P:238:THR:CB	3:P:239:PRO:HD3	2.48	0.40
2:O:292:THR:HG21	2:O:363:GLN:NE2	2.35	0.40
6:F:100:GLU:O	6:F:103:GLU:HB3	2.21	0.40
4:D:66:GLU:C	4:D:68:VAL:H	2.24	0.40
4:Q:238:ARG:NH1	5:R:5:VAL:HG22	2.36	0.40
1:N:159:GLN:HE21	1:N:237:THR:HB	1.87	0.40
4:D:167:GLU:C	4:D:169:LEU:H	2.25	0.40
8:H:65:ARG:O	8:H:69:VAL:HG23	2.21	0.40
5:R:144:CYS:HB2	5:R:158:CYS:SG	2.61	0.40
1:A:383:LEU:HD23	1:A:388:ARG:HA	2.03	0.40
1:A:122:LEU:HD11	1:A:186:ILE:HD12	2.02	0.40
7:T:30:PHE:O	7:T:35:PRO:CD	2.69	0.40
10:J:7:ARG:NH1	10:J:7:ARG:CB	2.85	0.40
1:N:282:ARG:HH21	9:V:36:UNK:HA	1.87	0.40
2:B:357:VAL:CG1	2:B:361:LYS:HE3	2.49	0.40
3:P:36:SER:O	3:P:40:VAL:HG23	2.21	0.40
2:B:71:LEU:CD1	2:B:144:LEU:HD23	2.51	0.40
2:B:353:THR:HG22	2:B:354:GLU:N	2.36	0.40
1:N:177:LEU:HD22	1:N:181:ASP:HB2	2.03	0.40
1:A:177:LEU:HD23	1:A:177:LEU:HA	1.94	0.40
1:N:39:VAL:HA	1:N:196:VAL:O	2.22	0.40
5:E:136:VAL:HG21	5:E:181:GLU:HG2	2.04	0.40
3:P:245:LEU:HD23	3:P:245:LEU:HA	1.80	0.40
1:A:156:THR:CG2	1:A:157:ALA:N	2.84	0.40
3:P:350:ILE:CG2	3:P:351:ILE:N	2.84	0.40
1:A:261:GLY:HA2	1:A:317:THR:O	2.21	0.40
4:Q:105:ASN:O	4:Q:106:ASN:CB	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:123:THR:HG21	3:C:190:ILE:HG13	2.03	0.40
2:O:403:ASP:C	2:O:405:VAL:H	2.25	0.40
1:A:361:LEU:O	1:A:364:ALA:HB3	2.22	0.40
2:B:437:ASP:OD1	2:B:437:ASP:O	2.39	0.40
1:N:35:CYS:HB2	1:N:200:ALA:O	2.21	0.40
9:V:70:LEU:HD23	9:V:70:LEU:C	2.42	0.40
4:D:116:ILE:CG2	4:D:117:VAL:N	2.85	0.40
4:D:237:TYR:HB2	6:F:60:PHE:CD1	2.57	0.40
2:B:280:GLY:HA3	2:B:293:SER:OG	2.21	0.40
1:A:4:TYR:OH	1:A:396:ASP:OD2	2.31	0.40
10:J:20:PHE:C	10:J:20:PHE:CD1	2.94	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	442/446 (99%)	391 (88%)	44 (10%)	7 (2%)	12 42
1	N	440/446 (99%)	380 (86%)	49 (11%)	11 (2%)	7 30
2	B	419/441 (95%)	337 (80%)	62 (15%)	20 (5%)	3 16
2	O	420/441 (95%)	351 (84%)	57 (14%)	12 (3%)	6 27
3	C	378/380 (100%)	332 (88%)	37 (10%)	9 (2%)	7 31
3	P	377/380 (99%)	322 (85%)	47 (12%)	8 (2%)	9 35
4	D	239/241 (99%)	212 (89%)	19 (8%)	8 (3%)	5 24
4	Q	239/241 (99%)	213 (89%)	15 (6%)	11 (5%)	3 16
5	E	194/196 (99%)	142 (73%)	32 (16%)	20 (10%)	1 3
5	R	194/196 (99%)	158 (81%)	23 (12%)	13 (7%)	1 8
6	F	99/110 (90%)	89 (90%)	9 (9%)	1 (1%)	19 56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
6	S	99/110 (90%)	88 (89%)	10 (10%)	1 (1%)	19 56
7	G	78/81 (96%)	63 (81%)	11 (14%)	4 (5%)	2 14
7	T	77/81 (95%)	60 (78%)	13 (17%)	4 (5%)	2 14
8	H	68/77 (88%)	57 (84%)	10 (15%)	1 (2%)	13 44
8	U	65/77 (84%)	48 (74%)	14 (22%)	3 (5%)	3 16
9	I	29/47 (62%)	20 (69%)	5 (17%)	4 (14%)	0 1
9	V	29/47 (62%)	23 (79%)	3 (10%)	3 (10%)	1 3
10	J	59/61 (97%)	46 (78%)	12 (20%)	1 (2%)	11 41
10	W	58/61 (95%)	45 (78%)	9 (16%)	4 (7%)	1 8
All	All	4003/4160 (96%)	3377 (84%)	481 (12%)	145 (4%)	4 22

All (145) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	21	ALA
2	B	22	GLU
2	B	24	LEU
2	B	26	ILE
2	B	29	LEU
2	B	171	ALA
2	B	227	ARG
2	B	228	SER
2	B	283	PRO
3	C	287	ASN
5	E	102	THR
5	E	115	SER
5	E	127	VAL
5	E	128	LYS
5	E	149	ASN
5	E	150	SER
5	E	177	PRO
7	G	79	ASN
9	I	63	ASP
1	N	433	ASP
2	O	26	ILE
2	O	171	ALA
2	O	228	SER
2	O	283	PRO
3	P	287	ASN

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Mol	Chain	Res	Type
4	Q	3	LEU
5	R	118	ARG
5	R	137	GLY
5	R	177	PRO
8	U	49	HIS
9	V	63	ASP
10	W	61	ALA
1	A	433	ASP
2	B	31	ASN
2	B	63	LEU
2	B	201	SER
2	B	221	GLU
2	B	269	ALA
2	B	420	GLY
5	E	130	PRO
5	E	137	GLY
5	E	151	GLY
5	E	163	SER
5	E	166	ASP
7	G	45	VAL
8	H	73	LEU
1	N	20	ASP
1	N	206	LYS
1	N	207	GLU
1	N	218	GLY
1	N	282	ARG
2	O	201	SER
4	Q	198	HIS
5	R	8	PRO
5	R	21	ALA
5	R	154	GLY
5	R	163	SER
5	R	166	ASP
5	R	188	VAL
6	S	83	TYR
7	T	3	HIS
7	T	33	ALA
7	T	45	VAL
8	U	73	LEU
1	A	282	ARG
1	A	388	ARG
2	B	30	PRO

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Mol	Chain	Res	Type
2	B	386	ALA
3	C	159	HIS
3	C	288	LYS
4	D	166	ASN
4	D	198	HIS
4	D	233	ARG
5	E	21	ALA
5	E	146	PRO
7	G	33	ALA
9	I	64	LEU
1	N	5	ALA
2	O	24	LEU
2	O	63	LEU
2	O	222	GLN
3	P	288	LYS
4	Q	2	GLU
4	Q	20	ALA
5	R	114	VAL
5	R	149	ASN
5	R	191	ASP
8	U	52	GLU
9	V	60	ALA
9	V	64	LEU
10	W	17	THR
2	B	389	SER
3	C	202	HIS
4	D	106	ASN
4	D	133	GLY
4	D	156	GLN
5	E	120	PRO
5	E	191	ASP
6	F	77	LYS
9	I	73	PRO
10	J	32	GLU
1	N	72	CYS
1	N	81	SER
1	N	388	ARG
3	P	156	TYR
3	P	202	HIS
4	Q	156	GLN
4	Q	162	PRO
4	Q	166	ASN

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Mol	Chain	Res	Type
4	Q	233	ARG
10	W	32	GLU
10	W	33	ARG
1	A	72	CYS
3	C	156	TYR
4	D	162	PRO
5	E	154	GLY
7	G	50	PRO
9	I	60	ALA
2	O	384	SER
2	O	389	SER
3	P	5	ILE
4	Q	133	GLY
4	Q	177	ALA
5	R	127	VAL
7	T	50	PRO
1	A	71	PRO
1	A	81	SER
1	A	443	TRP
2	B	190	GLN
3	C	3	PRO
4	D	38	SER
5	E	80	ASP
5	E	110	ALA
1	N	217	SER
3	P	157	ILE
4	Q	106	ASN
3	C	5	ILE
5	E	8	PRO
2	O	19	PRO
3	C	20	ILE
3	P	20	ILE
3	P	3	PRO
2	B	20	GLY
3	C	209	PRO
2	O	420	GLY

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%)	341 (93%)	24 (7%)	21 54
1	N	365/368 (99%)	341 (93%)	24 (7%)	21 54
2	B	331/347 (95%)	308 (93%)	23 (7%)	19 52
2	O	333/347 (96%)	314 (94%)	19 (6%)	25 60
3	C	328/329 (100%)	313 (95%)	15 (5%)	33 69
3	P	328/329 (100%)	314 (96%)	14 (4%)	35 71
4	D	200/200 (100%)	196 (98%)	4 (2%)	63 87
4	Q	200/200 (100%)	196 (98%)	4 (2%)	63 87
5	E	166/166 (100%)	158 (95%)	8 (5%)	31 67
5	R	165/166 (99%)	159 (96%)	6 (4%)	42 77
6	F	93/96 (97%)	90 (97%)	3 (3%)	46 79
6	S	93/96 (97%)	88 (95%)	5 (5%)	27 62
7	G	71/71 (100%)	67 (94%)	4 (6%)	26 61
7	T	70/71 (99%)	68 (97%)	2 (3%)	50 81
8	H	65/71 (92%)	64 (98%)	1 (2%)	72 90
8	U	63/71 (89%)	61 (97%)	2 (3%)	46 79
9	I	23/26 (88%)	20 (87%)	3 (13%)	5 20
9	V	23/26 (88%)	21 (91%)	2 (9%)	13 42
10	J	49/49 (100%)	46 (94%)	3 (6%)	23 57
10	W	47/49 (96%)	46 (98%)	1 (2%)	61 86
All	All	3378/3446 (98%)	3211 (95%)	167 (5%)	31 67

All (167) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	34	THR
1	A	49	ASN
1	A	58	PHE
1	A	86	PHE
1	A	102	LEU
1	A	106	MET
1	A	108	LYS

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Mol	Chain	Res	Type
1	A	146	THR
1	A	174	ILE
1	A	179	ARG
1	A	181	ASP
1	A	220	SER
1	A	226	ASP
1	A	248	LEU
1	A	274	ASN
1	A	307	PHE
1	A	342	TRP
1	A	344	ARG
1	A	350	THR
1	A	395	TRP
1	A	405	ARG
1	A	432	LEU
1	A	443	TRP
2	B	23	ASP
2	B	24	LEU
2	B	31	ASN
2	B	57	TYR
2	B	97	SER
2	B	104	LYS
2	B	114	ASP
2	B	154	SER
2	B	170	THR
2	B	239	TYR
2	B	248	ASN
2	B	250	HIS
2	B	270	ASN
2	B	283	PRO
2	B	296	TYR
2	B	304	THR
2	B	325	TYR
2	B	341	MET
2	B	343	GLN
2	B	344	LEU
2	B	376	GLN
2	B	402	ILE
2	B	424	MET
3	C	44	THR
3	C	81	ARG
3	C	82	ASN

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Mol	Chain	Res	Type
3	C	91	PHE
3	C	149	ASN
3	C	175	THR
3	C	184	PHE
3	C	216	SER
3	C	223	PRO
3	C	226	SER
3	C	240	PHE
3	C	243	LEU
3	C	277	PHE
3	C	367	PHE
3	C	380	TYR
4	D	43	MET
4	D	169	LEU
4	D	173	ASP
4	D	215	LEU
5	E	6	THR
5	E	31	ASP
5	E	52	LYS
5	E	61	SER
5	E	80	ASP
5	E	131	GLU
5	E	178	TYR
5	E	185	TYR
6	F	58	ARG
6	F	64	ARG
6	F	70	LEU
7	G	3	HIS
7	G	63	THR
7	G	79	ASN
7	G	80	ASP
8	H	49	HIS
9	I	68	ILE
9	I	70	LEU
9	I	71	ASN
10	J	22	LEU
10	J	59	TYR
10	J	64	GLU
1	N	3	THR
1	N	10	ASN
1	N	18	THR
1	N	49	ASN

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Mol	Chain	Res	Type
1	N	58	PHE
1	N	86	PHE
1	N	102	LEU
1	N	106	MET
1	N	108	LYS
1	N	174	ILE
1	N	179	ARG
1	N	181	ASP
1	N	220	SER
1	N	248	LEU
1	N	274	ASN
1	N	281	ASP
1	N	307	PHE
1	N	342	TRP
1	N	350	THR
1	N	376	CYS
1	N	395	TRP
1	N	405	ARG
1	N	432	LEU
1	N	443	TRP
2	O	22	GLU
2	O	31	ASN
2	O	57	TYR
2	O	104	LYS
2	O	114	ASP
2	O	154	SER
2	O	239	TYR
2	O	248	ASN
2	O	250	HIS
2	O	283	PRO
2	O	296	TYR
2	O	304	THR
2	O	325	TYR
2	O	341	MET
2	O	343	GLN
2	O	344	LEU
2	O	376	GLN
2	O	402	ILE
2	O	424	MET
3	P	44	THR
3	P	81	ARG
3	P	82	ASN

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Mol	Chain	Res	Type
3	P	149	ASN
3	P	175	THR
3	P	184	PHE
3	P	216	SER
3	P	226	SER
3	P	240	PHE
3	P	243	LEU
3	P	283	ARG
3	P	367	PHE
3	P	374	GLU
3	P	380	TYR
4	Q	43	MET
4	Q	76	GLU
4	Q	169	LEU
4	Q	215	LEU
5	R	6	THR
5	R	31	ASP
5	R	61	SER
5	R	178	TYR
5	R	185	TYR
5	R	188	VAL
6	S	13	MET
6	S	58	ARG
6	S	59	MET
6	S	64	ARG
6	S	70	LEU
7	T	3	HIS
7	T	63	THR
8	U	49	HIS
8	U	71	HIS
9	V	68	ILE
9	V	70	LEU
10	W	59	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (85) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	A	85	HIS
1	A	118	GLN
1	A	159	GLN
1	A	173	ASN

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Mol	Chain	Res	Type
1	A	274	ASN
1	A	289	HIS
1	A	308	GLN
1	A	339	GLN
2	B	31	ASN
2	B	153	GLN
2	B	156	GLN
2	B	197	ASN
2	B	247	GLN
2	B	248	ASN
2	B	270	ASN
2	B	276	GLN
2	B	297	GLN
2	B	329	GLN
2	B	343	GLN
2	B	362	ASN
2	B	363	GLN
3	C	9	HIS
3	C	69	HIS
3	C	82	ASN
3	C	207	ASN
3	C	313	GLN
3	C	332	ASN
3	C	342	GLN
4	D	35	GLN
4	D	50	ASN
4	D	148	HIS
5	E	3	ASN
5	E	57	GLN
5	E	122	HIS
5	E	149	ASN
5	E	164	HIS
7	G	23	GLN
7	G	44	GLN
7	G	73	ASN
8	H	71	HIS
8	H	75	ASN
9	I	71	ASN
1	N	10	ASN
1	N	49	ASN
1	N	85	HIS
1	N	118	GLN

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Mol	Chain	Res	Type
1	N	159	GLN
1	N	173	ASN
1	N	274	ASN
1	N	289	HIS
1	N	308	GLN
1	N	339	GLN
1	N	435	ASN
2	O	31	ASN
2	O	156	GLN
2	O	197	ASN
2	O	247	GLN
2	O	248	ASN
2	O	276	GLN
2	O	297	GLN
2	O	329	GLN
2	O	343	GLN
2	O	362	ASN
2	O	363	GLN
3	P	9	HIS
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	105	ASN
4	Q	148	HIS
5	R	3	ASN
5	R	57	GLN
5	R	164	HIS
5	R	186	GLN
7	T	12	HIS
7	T	23	GLN
7	T	44	GLN
7	T	73	ASN
7	T	79	ASN
8	U	75	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

29 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
12	IKR	C	2001	-	25,26,26	1.59	6 (24%)	31,35,35	1.21	3 (9%)
13	UQ	C	2002	-	19,19,63	2.49	11 (57%)	23,26,79	1.42	4 (17%)
14	CDL	C	2004	-	39,39,99	1.20	2 (5%)	41,51,111	1.15	4 (9%)
15	PEE	C	2007	-	48,48,50	1.31	7 (14%)	49,53,55	0.90	4 (8%)
15	PEE	C	2008	-	20,20,50	1.82	6 (30%)	21,25,55	0.65	0
16	GOL	C	2011	-	5,5,5	1.54	1 (20%)	5,5,5	0.80	0
11	HEM	C	501	3	30,50,50	2.81	9 (30%)	24,82,82	2.44	8 (33%)
11	HEM	C	502	3	30,50,50	2.45	7 (23%)	24,82,82	2.11	8 (33%)
14	CDL	D	2003	-	41,41,99	1.18	2 (4%)	43,53,111	1.10	2 (4%)
18	BOG	D	2009	-	20,20,20	1.07	1 (5%)	25,25,25	0.94	2 (8%)
18	BOG	D	2091	-	13,13,20	1.45	3 (23%)	18,18,25	1.12	2 (11%)
17	HEC	D	501	4	24,50,50	2.77	3 (12%)	19,82,82	3.53	8 (42%)
15	PEE	E	2005	-	49,49,50	1.42	9 (18%)	50,54,55	0.94	5 (10%)
19	FES	E	501	5	0,4,4	0.00	-	0,4,4	0.00	-
18	BOG	P	2010	-	12,12,20	1.52	4 (33%)	17,17,25	0.63	0
12	IKR	P	3001	-	25,26,26	1.41	4 (16%)	31,35,35	1.24	4 (12%)
13	UQ	P	3002	-	19,19,63	2.41	11 (57%)	23,26,79	1.42	4 (17%)
14	CDL	P	3004	-	39,39,99	1.22	2 (5%)	41,51,111	1.15	4 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	PEE	P	3007	-	48,48,50	1.28	6 (12%)	49,53,55	0.87	4 (8%)
15	PEE	P	3008	-	4,4,50	3.69	4 (100%)	6,6,55	0.53	0
16	GOL	P	3011	-	5,5,5	1.30	0	5,5,5	0.65	0
11	HEM	P	501	3	30,50,50	2.87	9 (30%)	24,82,82	2.37	8 (33%)
11	HEM	P	502	3	30,50,50	2.56	9 (30%)	24,82,82	2.29	8 (33%)
14	CDL	Q	3003	-	41,41,99	1.19	3 (7%)	43,53,111	1.08	2 (4%)
18	BOG	Q	3009	-	20,20,20	1.11	3 (15%)	25,25,25	1.02	2 (8%)
18	BOG	Q	3091	-	13,13,20	1.54	3 (23%)	18,18,25	1.06	2 (11%)
17	HEC	Q	501	4	24,50,50	2.26	3 (12%)	19,82,82	3.43	7 (36%)
15	PEE	R	3005	-	49,49,50	1.50	9 (18%)	50,54,55	0.96	5 (10%)
19	FES	R	501	5	0,4,4	0.00	-	0,4,4	0.00	-

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	IKR	C	2001	-	-	0/18/18/18	0/2/2/2
13	UQ	C	2002	-	-	0/11/35/87	0/1/1/1
14	CDL	C	2004	-	-	0/49/49/110	0/0/0/0
15	PEE	C	2007	-	-	0/52/52/54	0/0/0/0
15	PEE	C	2008	-	-	0/24/24/54	0/0/0/0
16	GOL	C	2011	-	-	0/4/4/4	0/0/0/0
11	HEM	C	501	3	-	0/10/54/54	0/0/8/8
11	HEM	C	502	3	-	0/10/54/54	0/0/8/8
14	CDL	D	2003	-	-	0/51/51/110	0/0/0/0
18	BOG	D	2009	-	-	0/11/31/31	0/1/1/1
18	BOG	D	2091	-	-	0/4/24/31	0/1/1/1
17	HEC	D	501	4	-	0/6/54/54	0/0/8/8
15	PEE	E	2005	-	-	0/53/53/54	0/0/0/0
19	FES	E	501	5	-	0/0/4/4	0/1/1/1
18	BOG	P	2010	-	-	0/2/22/31	0/1/1/1
12	IKR	P	3001	-	-	0/18/18/18	0/2/2/2
13	UQ	P	3002	-	-	0/11/35/87	0/1/1/1
14	CDL	P	3004	-	-	0/49/49/110	0/0/0/0
15	PEE	P	3007	-	-	0/52/52/54	0/0/0/0
15	PEE	P	3008	-	-	0/0/0/54	0/0/0/0
16	GOL	P	3011	-	-	0/4/4/4	0/0/0/0
11	HEM	P	501	3	-	0/10/54/54	0/0/8/8
11	HEM	P	502	3	-	0/10/54/54	0/0/8/8

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CDL	Q	3003	-	-	0/51/51/110	0/0/0/0
18	BOG	Q	3009	-	-	0/11/31/31	0/1/1/1
18	BOG	Q	3091	-	-	0/4/24/31	0/1/1/1
17	HEC	Q	501	4	-	0/6/54/54	0/0/8/8
15	PEE	R	3005	-	-	0/53/53/54	0/0/0/0
19	FES	R	501	5	-	0/0/4/4	0/1/1/1

All (137) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	D	501	HEC	C3B-C2B	-9.84	1.30	1.40
17	Q	501	HEC	C3B-C2B	-8.25	1.32	1.40
17	D	501	HEC	C3C-C2C	-7.60	1.32	1.40
11	P	501	HEM	C3B-C4B	-7.03	1.45	1.51
11	C	501	HEM	C3B-C4B	-6.88	1.45	1.51
11	C	501	HEM	C3B-CAB	-6.77	1.38	1.51
11	P	502	HEM	C3C-CAC	-6.56	1.39	1.51
11	P	502	HEM	C3B-CAB	-6.55	1.39	1.51
11	C	502	HEM	C3B-CAB	-6.54	1.39	1.51
11	C	502	HEM	C2D-C3D	-6.50	1.35	1.54
11	P	501	HEM	C3C-CAC	-6.28	1.39	1.51
11	C	501	HEM	C2D-C3D	-6.25	1.35	1.54
11	P	501	HEM	C3B-CAB	-6.23	1.39	1.51
11	C	501	HEM	C3C-CAC	-5.92	1.40	1.51
11	C	502	HEM	C3C-CAC	-5.90	1.40	1.51
11	P	502	HEM	C2D-C3D	-5.87	1.36	1.54
11	P	501	HEM	C2D-C3D	-5.68	1.37	1.54
17	Q	501	HEC	C3C-C2C	-5.36	1.35	1.40
11	P	501	HEM	C3D-C4D	-4.80	1.45	1.51
11	C	501	HEM	C3D-C4D	-3.88	1.46	1.51
11	C	502	HEM	C2C-C1C	-3.51	1.45	1.52
11	P	502	HEM	C2C-C1C	-3.19	1.46	1.52
11	P	502	HEM	C3B-C4B	-2.91	1.49	1.51
15	P	3007	PEE	C22-C21	-2.87	1.35	1.51
15	P	3007	PEE	C19-C18	-2.75	1.35	1.51
15	C	2007	PEE	C19-C18	-2.73	1.35	1.51
15	E	2005	PEE	C19-C18	-2.73	1.35	1.51
15	R	3005	PEE	C19-C18	-2.72	1.35	1.51
11	C	501	HEM	C2C-C1C	-2.72	1.47	1.52
15	R	3005	PEE	C22-C21	-2.71	1.35	1.51
11	P	501	HEM	C2C-C1C	-2.67	1.47	1.52
15	E	2005	PEE	C22-C21	-2.65	1.36	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	P	502	HEM	C3D-C4D	-2.64	1.48	1.51
15	C	2007	PEE	C22-C21	-2.60	1.36	1.51
12	C	2001	IKR	C1-I1	-2.11	2.04	2.10
11	C	502	HEM	C3D-C4D	-2.01	1.49	1.51
14	Q	3003	CDL	OA6-CA5	2.01	1.40	1.34
18	D	2091	BOG	C1-C2	2.02	1.58	1.52
15	P	3008	PEE	P-O2P	2.04	1.61	1.54
15	C	2007	PEE	C31-C30	2.06	1.56	1.50
18	Q	3009	BOG	C1-C2	2.07	1.58	1.52
14	Q	3003	CDL	CA3-CA4	2.07	1.56	1.50
12	C	2001	IKR	C20-C17	2.07	1.43	1.40
11	P	502	HEM	CAA-C2A	2.09	1.55	1.52
18	Q	3009	BOG	C4-C5	2.09	1.57	1.53
18	P	2010	BOG	C4-C3	2.10	1.57	1.52
13	P	3002	UQ	O2-C2	2.11	1.42	1.37
14	Q	3003	CDL	O1-C1	2.11	1.49	1.43
14	D	2003	CDL	OA6-CA5	2.15	1.40	1.34
13	P	3002	UQ	C8-C9	2.15	1.37	1.33
15	C	2007	PEE	C3-C2	2.18	1.56	1.50
15	P	3007	PEE	C3-C2	2.18	1.56	1.50
16	C	2011	GOL	O2-C2	2.20	1.50	1.43
14	D	2003	CDL	O1-C1	2.20	1.50	1.43
18	P	2010	BOG	C4-C5	2.23	1.57	1.53
18	D	2009	BOG	O5-C1	2.24	1.47	1.41
18	Q	3091	BOG	O5-C5	2.24	1.50	1.44
15	E	2005	PEE	C1-C2	2.25	1.57	1.50
14	C	2004	CDL	O1-C1	2.26	1.50	1.43
14	P	3004	CDL	O1-C1	2.28	1.50	1.43
15	E	2005	PEE	C3-C2	2.29	1.57	1.50
13	C	2002	UQ	C5-C4	2.32	1.56	1.47
13	C	2002	UQ	CM5-C5	2.32	1.55	1.50
13	P	3002	UQ	CM5-C5	2.32	1.55	1.50
18	P	2010	BOG	C1-C2	2.33	1.57	1.52
13	C	2002	UQ	C8-C9	2.34	1.37	1.33
12	P	3001	IKR	C21-C20	2.35	1.43	1.39
15	C	2008	PEE	C11-C10	2.38	1.57	1.50
15	R	3005	PEE	C31-C30	2.39	1.57	1.50
15	C	2008	PEE	C3-C2	2.39	1.57	1.50
11	C	501	HEM	C4C-NC	2.39	1.39	1.36
15	R	3005	PEE	C1-C2	2.40	1.57	1.50
13	P	3002	UQ	C7-C8	2.40	1.54	1.50
18	D	2091	BOG	C4-C5	2.40	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	D	501	HEC	C1A-NA	2.41	1.39	1.36
13	C	2002	UQ	C7-C8	2.44	1.54	1.50
18	Q	3009	BOG	O5-C1	2.44	1.48	1.41
13	P	3002	UQ	C5-C4	2.48	1.56	1.47
14	P	3004	CDL	CB3-CB4	2.53	1.57	1.50
15	R	3005	PEE	C3-C2	2.53	1.57	1.50
15	E	2005	PEE	C31-C30	2.56	1.58	1.50
12	P	3001	IKR	C24-C17	2.58	1.44	1.39
15	C	2008	PEE	C1-C2	2.59	1.58	1.50
13	C	2002	UQ	O2-C2	2.60	1.43	1.37
14	C	2004	CDL	CB3-CB4	2.62	1.58	1.50
18	D	2091	BOG	O5-C1	2.62	1.48	1.41
11	P	501	HEM	C1C-NC	2.63	1.39	1.36
13	P	3002	UQ	C3-C4	2.64	1.56	1.48
12	P	3001	IKR	C3-C4	2.66	1.43	1.38
18	Q	3091	BOG	C4-C5	2.67	1.58	1.53
15	C	2007	PEE	O2-C10	2.70	1.42	1.34
13	P	3002	UQ	C2-C1	2.71	1.56	1.48
15	P	3007	PEE	P-O1P	2.72	1.61	1.51
15	P	3008	PEE	P-O4P	2.72	1.64	1.54
15	P	3008	PEE	P-O3P	2.75	1.64	1.54
15	P	3007	PEE	O2-C10	2.77	1.42	1.34
18	Q	3091	BOG	O5-C1	2.78	1.48	1.41
12	C	2001	IKR	C3-C4	2.79	1.44	1.38
12	C	2001	IKR	C21-C20	2.81	1.44	1.39
18	P	2010	BOG	O5-C1	2.82	1.48	1.43
15	E	2005	PEE	P-O1P	2.84	1.61	1.51
12	P	3001	IKR	C40-C2	2.87	1.56	1.51
15	E	2005	PEE	C11-C10	2.88	1.59	1.50
15	C	2007	PEE	P-O1P	2.88	1.61	1.51
13	C	2002	UQ	C2-C1	2.89	1.57	1.48
12	C	2001	IKR	C24-C17	2.92	1.44	1.39
15	C	2008	PEE	P-O1P	2.96	1.62	1.51
17	Q	501	HEC	C1A-NA	2.96	1.40	1.36
15	R	3005	PEE	P-O1P	2.97	1.62	1.51
13	C	2002	UQ	C3-C4	3.01	1.57	1.48
15	C	2008	PEE	O3-C30	3.05	1.42	1.33
13	P	3002	UQ	O3-C3	3.07	1.45	1.37
15	P	3007	PEE	O3-C30	3.10	1.42	1.33
15	C	2007	PEE	O3-C30	3.14	1.42	1.33
15	R	3005	PEE	O3-C30	3.16	1.42	1.33
11	C	501	HEM	CBB-CAB	3.16	1.47	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	R	3005	PEE	C11-C10	3.20	1.60	1.50
15	E	2005	PEE	O2-C10	3.21	1.43	1.34
15	E	2005	PEE	O3-C30	3.21	1.43	1.33
15	C	2008	PEE	O2-C10	3.27	1.44	1.34
12	C	2001	IKR	C40-C2	3.42	1.57	1.51
13	C	2002	UQ	O3-C3	3.45	1.46	1.37
13	C	2002	UQ	C6-C5	3.48	1.43	1.35
11	P	502	HEM	CBC-CAC	3.55	1.49	1.29
15	R	3005	PEE	O2-C10	3.62	1.45	1.34
13	P	3002	UQ	C6-C1	3.63	1.56	1.46
11	C	502	HEM	CBC-CAC	3.63	1.50	1.29
13	P	3002	UQ	C6-C5	3.70	1.44	1.35
11	C	502	HEM	CBB-CAB	3.86	1.51	1.29
13	C	2002	UQ	C6-C1	3.95	1.57	1.46
11	P	501	HEM	CBB-CAB	3.98	1.52	1.29
11	P	502	HEM	CBB-CAB	3.99	1.52	1.29
11	C	501	HEM	CBC-CAC	4.00	1.52	1.29
11	P	501	HEM	CBC-CAC	4.02	1.52	1.29
13	C	2002	UQ	C7-C6	4.68	1.59	1.51
13	P	3002	UQ	C7-C6	5.02	1.60	1.51
15	P	3008	PEE	P-O1P	5.95	1.62	1.50

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	D	501	HEC	CBC-CAC-C3C	-10.65	103.68	127.35
17	Q	501	HEC	CBC-CAC-C3C	-10.46	104.10	127.35
17	D	501	HEC	CBB-CAB-C3B	-5.90	114.25	127.35
17	Q	501	HEC	CBB-CAB-C3B	-5.65	114.81	127.35
11	C	501	HEM	CBA-CAA-C2A	-5.57	102.54	112.53
11	P	501	HEM	CBA-CAA-C2A	-4.35	104.73	112.53
11	P	502	HEM	C3B-CAB-CBB	-4.07	118.22	124.46
13	P	3002	UQ	C7-C6-C1	-3.63	114.29	118.56
13	C	2002	UQ	C7-C6-C1	-3.53	114.41	118.56
12	P	3001	IKR	C40-C2-C3	-3.21	113.52	119.49
14	P	3004	CDL	CB4-OB6-CB5	-3.19	110.25	117.89
14	C	2004	CDL	CB4-OB6-CB5	-3.12	110.40	117.89
17	D	501	HEC	CAA-C2A-C3A	-3.08	120.22	129.00
12	C	2001	IKR	C40-C2-C3	-2.94	114.02	119.49
11	C	502	HEM	C3B-CAB-CBB	-2.85	120.09	124.46
14	P	3004	CDL	CA6-CA4-CA3	-2.81	105.50	112.07
14	D	2003	CDL	CB4-OB6-CB5	-2.78	111.21	117.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	P	3002	UQ	C10-C9-C8	-2.78	118.05	123.50
13	C	2002	UQ	C10-C9-C8	-2.75	118.11	123.50
11	P	501	HEM	C3C-CAC-CBC	-2.73	120.27	124.46
17	Q	501	HEC	CAA-C2A-C3A	-2.72	121.24	129.00
14	C	2004	CDL	CA4-OA6-CA5	-2.71	111.38	117.89
14	C	2004	CDL	CA6-CA4-CA3	-2.55	106.11	112.07
14	D	2003	CDL	CA6-CA4-CA3	-2.54	106.12	112.07
14	Q	3003	CDL	CB4-OB6-CB5	-2.52	111.85	117.89
12	P	3001	IKR	O31-C30-C29	-2.51	109.19	111.73
12	C	2001	IKR	O31-C30-C29	-2.50	109.20	111.73
14	Q	3003	CDL	CA6-CA4-CA3	-2.45	106.34	112.07
14	P	3004	CDL	CA4-OA6-CA5	-2.34	112.26	117.89
11	C	501	HEM	CMA-C3A-C4A	-2.08	124.93	128.36
12	P	3001	IKR	O15-C4-C5	2.01	119.73	115.25
17	D	501	HEC	CBD-CAD-C3D	2.08	116.26	112.53
11	C	502	HEM	C3B-C4B-CHC	2.10	126.12	123.16
15	E	2005	PEE	O3-C3-C2	2.10	114.36	108.69
13	P	3002	UQ	C11-C9-C8	2.17	125.58	120.74
17	Q	501	HEC	CBD-CAD-C3D	2.18	116.43	112.53
15	P	3007	PEE	C22-C21-C20	2.21	125.97	114.53
15	R	3005	PEE	O3-C3-C2	2.22	114.66	108.69
13	C	2002	UQ	C11-C9-C8	2.28	125.82	120.74
14	C	2004	CDL	OB6-CB4-CB3	2.30	116.45	108.36
14	P	3004	CDL	OB6-CB4-CB3	2.33	116.58	108.36
12	C	2001	IKR	O31-C30-O36	2.38	128.31	123.56
18	Q	3091	BOG	O1-C1-C2	2.39	111.03	108.21
15	R	3005	PEE	C23-C22-C21	2.40	126.94	114.53
15	P	3007	PEE	C23-C22-C21	2.41	126.98	114.53
15	C	2007	PEE	C22-C21-C20	2.42	127.04	114.53
18	D	2009	BOG	O1-C1-C2	2.43	111.10	108.04
15	E	2005	PEE	C23-C22-C21	2.43	127.09	114.53
15	P	3007	PEE	C19-C18-C17	2.49	127.38	114.53
15	R	3005	PEE	C22-C21-C20	2.52	127.52	114.53
15	C	2007	PEE	C19-C18-C17	2.54	127.64	114.53
12	P	3001	IKR	O31-C30-O36	2.54	128.62	123.56
15	C	2007	PEE	C23-C22-C21	2.55	127.69	114.53
15	E	2005	PEE	C19-C18-C17	2.56	127.73	114.53
15	E	2005	PEE	C22-C21-C20	2.56	127.77	114.53
18	D	2091	BOG	O1-C1-C2	2.58	111.26	108.21
18	Q	3009	BOG	O1-C1-C2	2.66	111.39	108.04
17	D	501	HEC	CMC-C2C-C1C	2.70	132.82	128.36
15	R	3005	PEE	C19-C18-C17	2.70	128.46	114.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	C	501	HEM	CMD-C2D-C3D	2.70	126.31	114.35
15	R	3005	PEE	C20-C19-C18	2.71	128.51	114.53
15	P	3007	PEE	C20-C19-C18	2.72	128.58	114.53
11	P	502	HEM	CMD-C2D-C3D	2.73	126.44	114.35
15	E	2005	PEE	C20-C19-C18	2.75	128.73	114.53
11	C	502	HEM	CMD-C2D-C3D	2.76	126.56	114.35
15	C	2007	PEE	C20-C19-C18	2.81	129.04	114.53
11	P	501	HEM	CMD-C2D-C3D	2.85	126.94	114.35
17	Q	501	HEC	CAD-C3D-C4D	2.93	130.19	127.01
11	P	502	HEM	CBA-CAA-C2A	3.05	117.99	112.53
11	C	501	HEM	C2D-C3D-C4D	3.06	106.69	101.50
11	P	501	HEM	C2D-C3D-C4D	3.15	106.84	101.50
17	D	501	HEC	CBA-CAA-C2A	3.17	118.22	112.53
18	Q	3091	BOG	C1'-O1-C1	3.27	118.64	113.29
11	P	502	HEM	CAD-C3D-C2D	3.28	122.66	113.22
11	C	502	HEM	CMC-C2C-C3C	3.31	124.79	116.53
18	D	2009	BOG	C1'-O1-C1	3.31	119.74	113.94
11	C	502	HEM	C2D-C3D-C4D	3.32	107.13	101.50
11	C	502	HEM	CAD-C3D-C2D	3.37	122.91	113.22
11	C	501	HEM	CAD-C3D-C2D	3.37	122.92	113.22
18	D	2091	BOG	C1'-O1-C1	3.40	118.86	113.29
11	P	502	HEM	C2D-C3D-C4D	3.43	107.31	101.50
11	P	501	HEM	CAD-C3D-C2D	3.44	123.11	113.22
18	Q	3009	BOG	C1'-O1-C1	3.70	120.41	113.94
17	D	501	HEC	CAD-C3D-C4D	3.84	131.18	127.01
11	C	502	HEM	CMB-C2B-C3B	3.85	126.13	116.53
13	P	3002	UQ	C8-C7-C6	3.95	123.50	111.64
13	C	2002	UQ	C8-C7-C6	4.07	123.86	111.64
17	Q	501	HEC	CBA-CAA-C2A	4.13	119.93	112.53
11	P	502	HEM	CMB-C2B-C3B	4.36	127.42	116.53
11	C	501	HEM	CMC-C2C-C3C	4.51	127.79	116.53
11	C	501	HEM	CMB-C2B-C3B	4.59	127.98	116.53
11	P	502	HEM	CMC-C2C-C3C	4.60	128.01	116.53
11	P	501	HEM	CMC-C2C-C3C	4.64	128.10	116.53
11	C	502	HEM	CAD-C3D-C4D	4.73	129.14	112.47
11	P	502	HEM	CAD-C3D-C4D	4.75	129.21	112.47
11	P	501	HEM	CAD-C3D-C4D	4.96	129.97	112.47
11	C	501	HEM	CAD-C3D-C4D	5.08	130.39	112.47
11	P	501	HEM	CMB-C2B-C3B	5.15	129.38	116.53
17	D	501	HEC	CAA-C2A-C1A	6.10	133.63	127.01
17	Q	501	HEC	CAA-C2A-C1A	6.32	133.87	127.01

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

22 monomers are involved in 52 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	C	2001	IKR	4	0
13	C	2002	UQ	6	0
14	C	2004	CDL	1	0
15	C	2007	PEE	1	0
11	C	501	HEM	3	0
11	C	502	HEM	4	0
18	D	2009	BOG	1	0
17	D	501	HEC	2	0
19	E	501	FES	2	0
18	P	2010	BOG	1	0
12	P	3001	IKR	3	0
13	P	3002	UQ	5	0
14	P	3004	CDL	2	0
15	P	3007	PEE	2	0
16	P	3011	GOL	2	0
11	P	501	HEM	2	0
11	P	502	HEM	3	0
14	Q	3003	CDL	2	0
18	Q	3009	BOG	1	0
17	Q	501	HEC	2	0
15	R	3005	PEE	1	0
19	R	501	FES	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	444/446 (99%)	-0.20	3 (0%) 89 75	39, 74, 106, 125	0
1	N	442/446 (99%)	-0.10	4 (0%) 85 69	43, 79, 111, 119	0
2	B	421/441 (95%)	-0.05	6 (1%) 78 57	63, 90, 121, 156	0
2	O	422/441 (95%)	-0.11	8 (1%) 70 45	50, 85, 115, 134	0
3	C	380/380 (100%)	-0.37	4 (1%) 82 63	23, 45, 98, 135	0
3	P	379/380 (99%)	-0.22	5 (1%) 79 59	32, 68, 104, 128	0
4	D	241/241 (100%)	-0.38	0 100 100	37, 51, 89, 114	0
4	Q	241/241 (100%)	-0.10	1 (0%) 93 84	55, 85, 118, 130	0
5	E	196/196 (100%)	1.31	63 (32%) 1 0	39, 140, 179, 186	125 (63%)
5	R	196/196 (100%)	0.72	38 (19%) 1 0	51, 99, 146, 165	0
6	F	101/110 (91%)	-0.54	0 100 100	38, 52, 70, 90	0
6	S	101/110 (91%)	-0.17	1 (0%) 84 66	62, 84, 126, 151	0
7	G	80/81 (98%)	-0.25	0 100 100	39, 61, 118, 127	0
7	T	79/81 (97%)	0.10	7 (8%) 12 4	55, 91, 154, 161	0
8	H	70/77 (90%)	-0.36	1 (1%) 78 57	52, 74, 95, 133	0
8	U	67/77 (87%)	0.53	6 (8%) 12 4	103, 131, 152, 157	0
9	I	31/47 (65%)	1.69	11 (35%) 0 0	92, 128, 164, 167	0
9	V	31/47 (65%)	1.59	10 (32%) 1 0	87, 119, 167, 170	0
10	J	61/61 (100%)	-0.24	1 (1%) 74 52	46, 63, 107, 143	0
10	W	60/61 (98%)	0.18	1 (1%) 73 49	65, 83, 120, 129	0
All	All	4043/4160 (97%)	-0.03	170 (4%) 40 18	23, 77, 138, 186	125 (3%)

All (170) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	E	113	ASP	11.3
5	E	107	ASN	8.6
9	I	51	CYS	8.1
5	E	167	ALA	6.8
5	E	98	VAL	6.5
5	E	112	VAL	6.3
5	E	174	GLY	6.3
5	E	168	SER	6.3
5	R	114	VAL	6.2
9	V	56	SER	5.8
5	E	86	ASN	5.8
5	E	101	ARG	5.5
5	E	84	GLY	5.5
5	E	180	LEU	5.5
5	E	102	THR	5.5
5	E	126	ARG	5.3
5	R	112	VAL	5.1
5	R	111	GLU	5.1
5	E	87	VAL	5.1
5	E	105	GLU	5.0
5	E	135	LEU	4.8
5	E	106	ILE	4.8
5	E	169	GLY	4.6
9	V	57	GLY	4.6
5	E	115	SER	4.5
5	E	148	ALA	4.4
9	I	50	LEU	4.4
5	R	122	HIS	4.4
5	E	114	VAL	4.3
5	E	99	ARG	4.3
5	R	98	VAL	4.3
5	E	104	ALA	4.2
8	U	13	LEU	4.2
5	E	109	GLU	4.2
5	R	86	ASN	4.1
5	E	187	PHE	4.0
5	E	120	PRO	4.0
2	B	350	GLY	3.9
5	E	173	LYS	3.9
2	O	222	GLN	3.9
7	T	74	PRO	3.8
2	B	225	ASN	3.8
9	V	63	ASP	3.8

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Mol	Chain	Res	Type	RSRZ
5	R	113	ASP	3.7
3	C	4	ASN	3.7
5	E	103	GLN	3.7
5	E	157	TYR	3.7
5	E	134	ILE	3.7
5	R	120	PRO	3.7
5	E	116	LYS	3.6
5	E	81	ILE	3.6
5	E	108	GLN	3.6
5	E	149	ASN	3.5
7	T	73	ASN	3.5
5	R	124	LEU	3.4
5	E	133	VAL	3.4
5	R	121	GLN	3.4
5	E	171	ILE	3.4
5	R	186	GLN	3.4
5	E	111	GLU	3.4
5	R	130	PRO	3.4
2	O	350	GLY	3.4
2	B	227	ARG	3.3
9	I	53	GLU	3.3
5	E	117	LEU	3.3
5	R	172	ARG	3.3
1	A	69	LYS	3.2
10	J	63	GLU	3.2
9	I	63	ASP	3.2
5	R	87	VAL	3.2
5	E	100	HIS	3.1
5	E	110	ALA	3.1
2	B	228	SER	3.1
5	R	156	TYR	3.1
5	R	127	VAL	3.1
5	E	188	VAL	3.1
2	O	19	PRO	3.1
2	O	347	ALA	3.1
5	R	109	GLU	3.1
5	R	133	VAL	3.0
5	R	184	THR	3.0
5	E	78	LEU	3.0
5	R	89	PHE	3.0
9	I	47	ARG	2.9
5	E	190	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	N	217	SER	2.9
5	E	165	TYR	2.9
9	I	52	ARG	2.9
9	V	77	ARG	2.9
1	N	66	GLY	2.9
2	B	402	ILE	2.9
5	E	97	PHE	2.9
3	C	7	LYS	2.9
5	E	125	ASP	2.8
7	T	78	GLU	2.8
5	E	124	LEU	2.8
5	E	183	PRO	2.8
5	R	88	ALA	2.8
9	V	53	GLU	2.8
5	R	134	ILE	2.8
7	T	2	ILE	2.8
5	R	154	GLY	2.7
9	I	61	ARG	2.7
5	E	156	TYR	2.7
2	O	352	VAL	2.7
9	I	77	ARG	2.7
5	R	115	SER	2.7
9	V	61	ARG	2.7
9	V	59	SER	2.6
3	C	8	SER	2.6
10	W	45	HIS	2.6
5	R	76	ILE	2.6
7	T	80	ASP	2.6
3	P	156	TYR	2.5
5	R	96	LEU	2.5
8	U	44	VAL	2.5
5	E	146	PRO	2.5
9	I	62	ARG	2.5
5	E	85	LYS	2.5
5	R	97	PHE	2.5
5	E	150	SER	2.5
3	P	6	ARG	2.5
5	R	85	LYS	2.5
8	U	50	THR	2.5
5	E	163	SER	2.5
2	O	410	VAL	2.5
9	I	55	MET	2.4

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Mol	Chain	Res	Type	RSRZ
3	P	4	ASN	2.4
5	E	122	HIS	2.4
6	S	11	ARG	2.4
5	E	121	GLN	2.4
5	R	108	GLN	2.4
5	R	125	ASP	2.4
3	P	7	LYS	2.4
5	R	128	LYS	2.4
5	E	147	ILE	2.4
9	V	55	MET	2.4
8	U	12	GLU	2.4
5	E	79	SER	2.4
9	I	56	SER	2.4
5	R	135	LEU	2.4
5	E	175	PRO	2.4
5	R	81	ILE	2.3
5	E	83	GLU	2.3
8	U	39	LEU	2.3
4	Q	139	ALA	2.3
5	R	110	ALA	2.3
5	R	165	TYR	2.3
5	E	159	PRO	2.3
1	A	219	VAL	2.3
7	T	77	TYR	2.2
5	E	89	PHE	2.2
9	V	58	ARG	2.2
3	P	157	ILE	2.2
2	B	33	LEU	2.2
8	U	14	VAL	2.2
5	E	145	VAL	2.2
1	A	217	SER	2.2
2	O	23	ASP	2.2
5	R	171	ILE	2.2
1	N	177	LEU	2.2
9	V	62	ARG	2.1
8	H	71	HIS	2.1
5	E	158	CYS	2.1
5	R	117	LEU	2.1
5	R	116	LYS	2.1
1	N	65	LYS	2.1
7	T	75	ALA	2.0
2	O	374	THR	2.0

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Mol	Chain	Res	Type	RSRZ
3	C	1	MET	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
15	PEE	E	2005	50/51	0.82	0.42	6.54	79,91,105,106	0
15	PEE	P	3007	49/51	0.89	0.37	4.39	68,91,107,109	0
14	CDL	Q	3003	42/100	0.76	0.34	4.21	120,141,152,153	0
15	PEE	C	2008	21/51	0.67	0.39	3.95	132,138,141,142	0
16	GOL	C	2011	6/6	0.90	0.27	3.92	54,56,58,60	0
16	GOL	P	3011	6/6	0.90	0.32	3.73	79,79,79,80	0
14	CDL	P	3004	40/100	0.83	0.33	3.23	111,116,122,123	0
15	PEE	C	2007	49/51	0.93	0.29	3.23	49,59,88,90	0
15	PEE	R	3005	50/51	0.79	0.35	3.14	80,99,106,107	0
13	UQ	C	2002	19/63	0.88	0.28	2.76	85,89,90,90	0
18	BOG	P	2010	12/20	0.57	0.42	2.75	162,165,167,167	0
14	CDL	D	2003	42/100	0.80	0.29	2.50	112,121,125,126	0
18	BOG	Q	3009	20/20	0.90	0.32	2.40	71,99,102,102	0
13	UQ	P	3002	19/63	0.85	0.29	2.24	97,111,114,115	0
18	BOG	D	2009	20/20	0.93	0.29	2.11	51,76,80,81	0
14	CDL	C	2004	40/100	0.89	0.25	1.22	72,82,99,101	0
11	HEM	C	501	43/43	0.98	0.21	0.58	30,37,43,45	0
11	HEM	P	501	43/43	0.98	0.21	0.46	46,50,57,60	0
11	HEM	P	502	43/43	0.97	0.21	0.45	40,47,59,62	0
17	HEC	Q	501	43/43	0.96	0.23	0.21	68,71,76,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
12	IKR	P	3001	25/25	0.98	0.19	0.01	66,67,76,78	0
17	HEC	D	501	43/43	0.98	0.18	-0.02	38,42,46,48	0
11	HEM	C	502	43/43	0.98	0.19	-0.20	24,31,37,44	0
12	IKR	C	2001	25/25	0.99	0.16	-0.97	38,40,44,54	0
19	FES	R	501	4/4	0.98	0.09	-1.56	88,90,91,91	0
19	FES	E	501	4/4	0.95	0.11	-2.15	151,151,152,152	4
18	BOG	D	2091	13/20	0.50	0.63	-	167,171,171,171	0
15	PEE	P	3008	5/51	0.80	0.26	-	140,140,140,140	0
18	BOG	Q	3091	13/20	0.31	0.77	-	194,197,197,198	0

6.5 Other polymers (i)

There are no such residues in this entry.