Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 09:07 AM GMT

PDB ID	:	3H1L
Title	:	Chicken cytochrome BC1 complex with ascochlorin bound at QO and QI sites
Authors	:	Berry, E.A.; Huang, L.S.; Minagawa, N.
Deposited on	:	2009-04-12
Resolution	:	3.21 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:

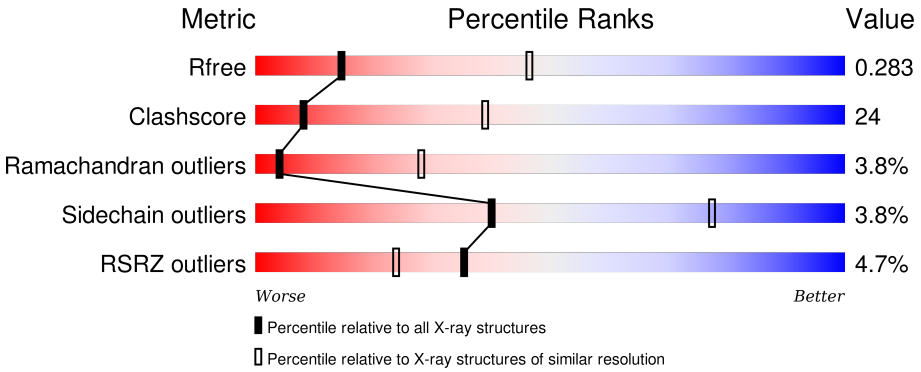
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.21 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	1095 (3.26-3.18)
Clashscore	102246	1046 (3.24-3.20)
Ramachandran outliers	100387	1026 (3.24-3.20)
Sidechain outliers	100360	1025 (3.24-3.20)
RSRZ outliers	91569	1100 (3.26-3.18)

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	3% 57% 39%
1	N	446	3% 57% 38% 5%
2	B	441	4% 47% 43% 5% 5%
2	O	441	4% 49% 41% 5%
3	C	380	2% 58% 39%

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Mol	Chain	Length	Quality of chain
3	P	380	2% 54% 42%
4	D	241	% 66% 33%
4	Q	241	2% 62% 37%
5	E	196	17% 48% 47%
5	R	196	9% 52% 44%
6	F	110	63% 26% 8%
6	S	110	4% 53% 35% 8%
7	G	81	% 46% 46% 9%
7	T	81	15% 43% 44% 10%
8	H	77	% 56% 32% 9%
8	U	77	8% 45% 40% 13%
9	I	47	17% 53% 38% 6%
9	V	47	21% 40% 49% 6%
10	J	61	2% 56% 38% 7%
10	W	61	11% 48% 44% 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
11	PEE	C	2007	-	-	-	X
11	PEE	E	2005	-	-	-	X
11	PEE	P	3008	-	X	-	-
11	PEE	R	3005	-	-	-	X
12	UNL	A	3016	-	-	-	X
12	UNL	P	3103	-	-	-	X
12	UNL	R	2103	-	-	-	X
15	CDL	P	3003	-	-	-	X
16	GOL	C	2011	-	-	-	X
16	GOL	P	3011	-	-	-	X
18	BOG	D	2009	-	-	-	X

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 32657 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	443	Total	C	N	O	S	0	0	1
			3440	2155	606	658	21			
1	N	442	Total	C	N	O	S	0	0	0
			3437	2154	605	657	21			

- Molecule 2 is a protein called MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 2.

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

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	380	Total	C	N	O	S	0	0	0
			3020	2024	478	505	13			
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 Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	196	Total	C	N	O	S	0	0	0
			1513	952	263	292	6			
5	R	196	Total	C	N	O	S	0	0	0
			1513	952	263	292	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	571	160	157	3			
6	S	101	Total	C	N	O	S	0	0	0
			891	571	160	157	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	81	Total	C	N	O	0	0	0
			676	439	120	117			
7	T	79	Total	C	N	O	0	0	0
			658	430	117	111			

- 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			

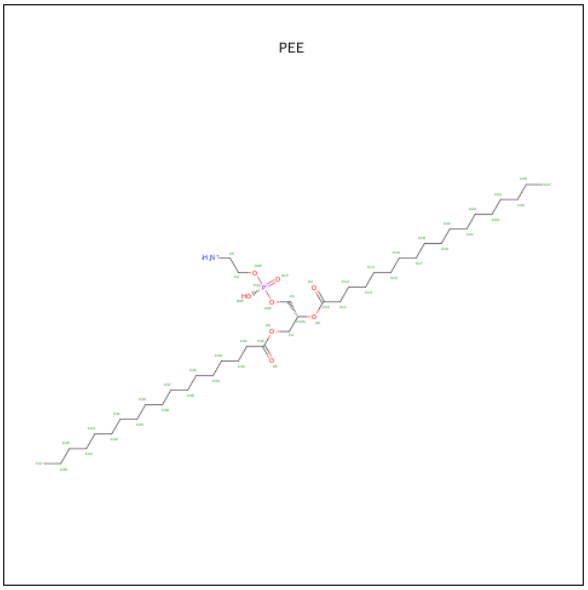
- Molecule 9 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	46	Total	C	N	O	S	0	0	0
			285	169	58	56	2			
9	V	44	Total	C	N	O	S	0	0	1
			275	164	56	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 497 321 87 89	0	0	0
10	W	59	Total C N O 478 311 85 82	0	0	0

- Molecule 11 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PEE) (formula: $C_{41}H_{83}NO_8P$).



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

- Molecule 12 is UNKNOWN LIGAND (three-letter code: UNL) (formula:).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	P	5	Total O 5 5	0	0

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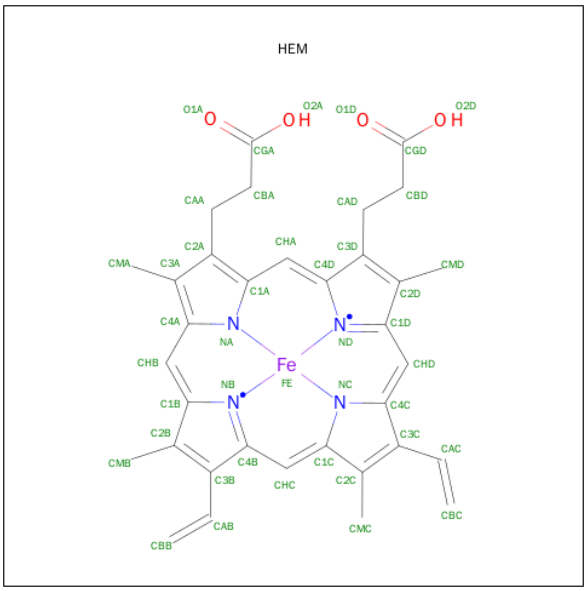
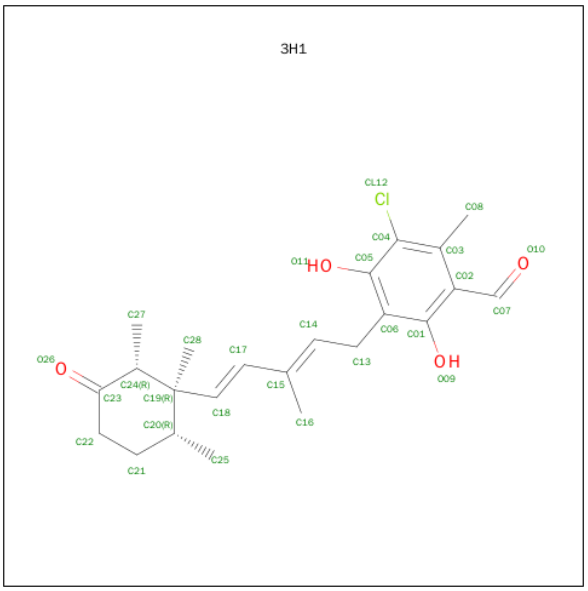
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	R	1	Total O 1 1	0	0
12	A	1	Total O 1 1	0	0
12	C	4	Total O 4 4	0	0
12	E	1	Total O 1 1	0	0

- Molecule 13 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



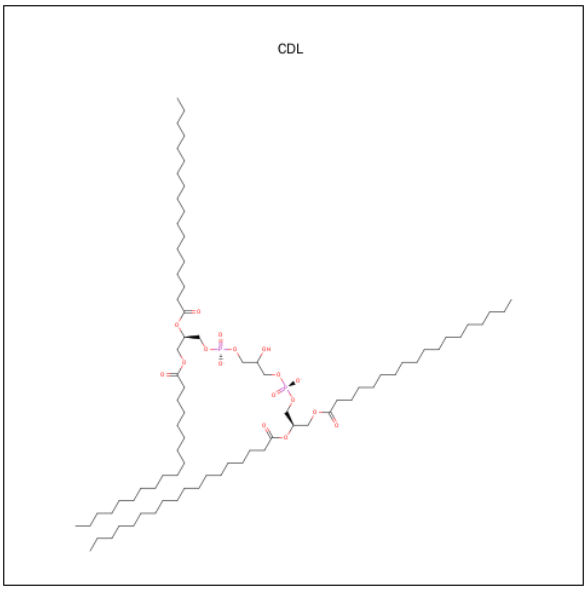
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	C	1	Total C Fe N O 43 34 1 4 4	0	0
13	C	1	Total C Fe N O 43 34 1 4 4	0	0
13	P	1	Total C Fe N O 43 34 1 4 4	0	0
13	P	1	Total C Fe N O 43 34 1 4 4	0	0

- Molecule 14 is 3-CHLORO-4,6-DIHYDROXY-2-METHYL-5-{(2E,4E)-3-METHYL-5-[(1R, 2R,6R)-1,2,6-TRIMETHYL-3-OXOCYCLOHEXYL]PENTA-2,4-DIEN-1-YL}BENZALDE HYDE (three-letter code: 3H1) (formula: $C_{23}H_{29}ClO_4$).



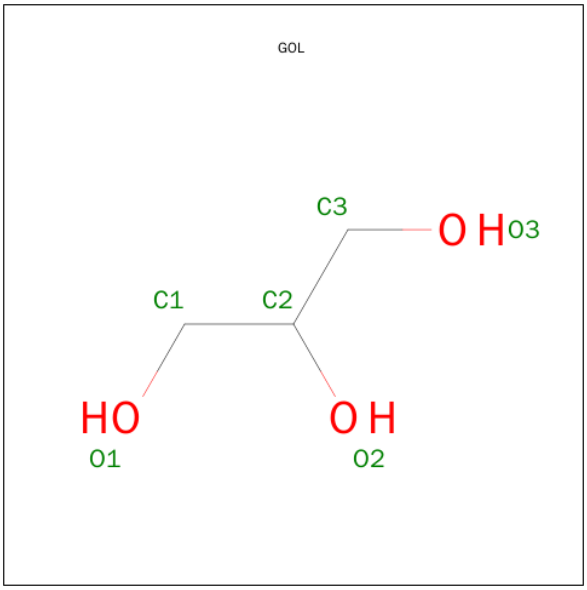
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	C	1	Total	C	Cl	O	0	0
			28	23	1	4		
14	C	1	Total	C	Cl	O	0	0
			28	23	1	4		
14	P	1	Total	C	Cl	O	0	0
			28	23	1	4		
14	P	1	Total	C	Cl	O	0	0
			28	23	1	4		

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



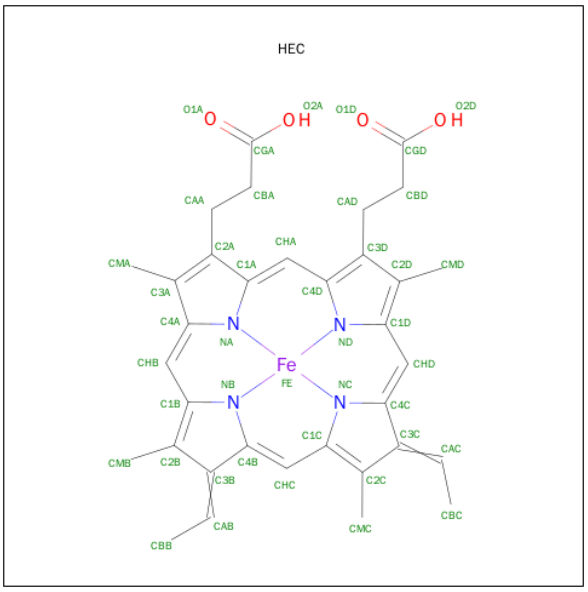
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	C	1	Total C O P 50 31 17 2	0	0
15	G	1	Total C O P 40 21 17 2	0	0
15	P	1	Total C O P 50 31 17 2	0	0
15	T	1	Total C O P 40 21 17 2	0	0

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



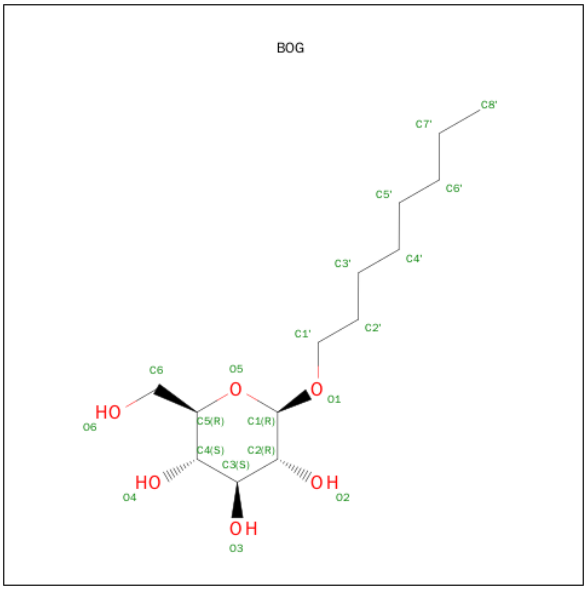
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	C	1	Total C O 6 3 3	0	0
16	P	1	Total C O 6 3 3	0	0

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



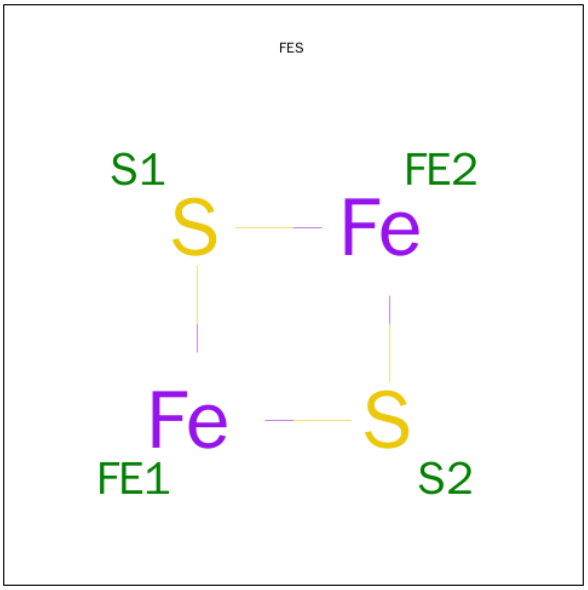
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
17	Q	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- 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	0	0
			20	14	6		
18	R	1	Total	C	O	0	0
			20	14	6		

- 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.

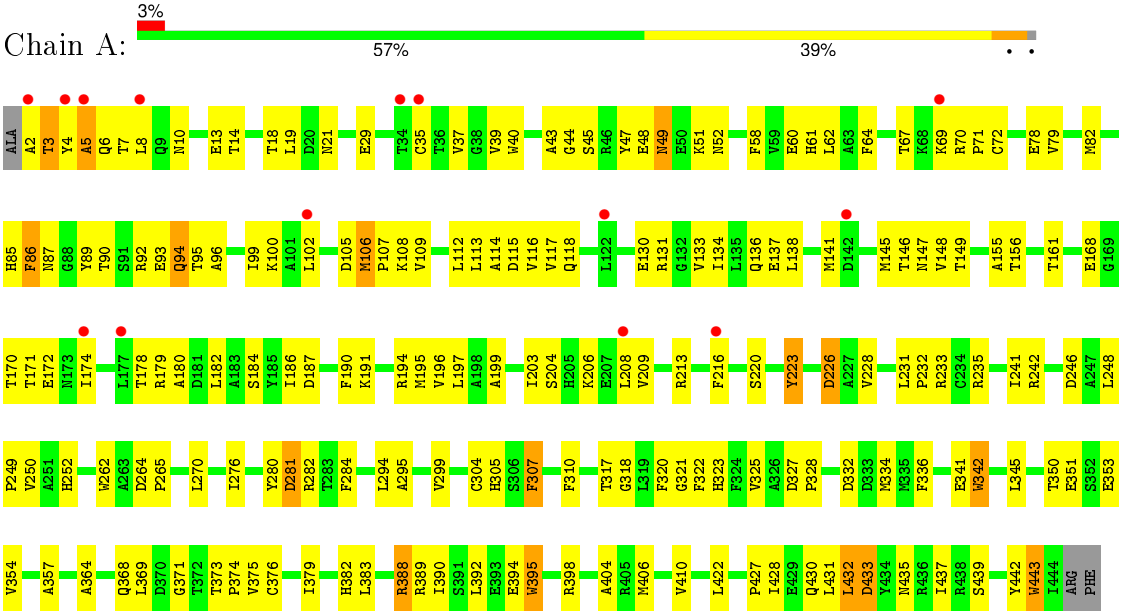
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
20	B	1	Total O 1 1	0	0
20	C	6	Total O 6 6	0	0
20	P	6	Total O 6 6	0	0
20	U	1	Total O 1 1	0	0

3 Residue-property plots (i)

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

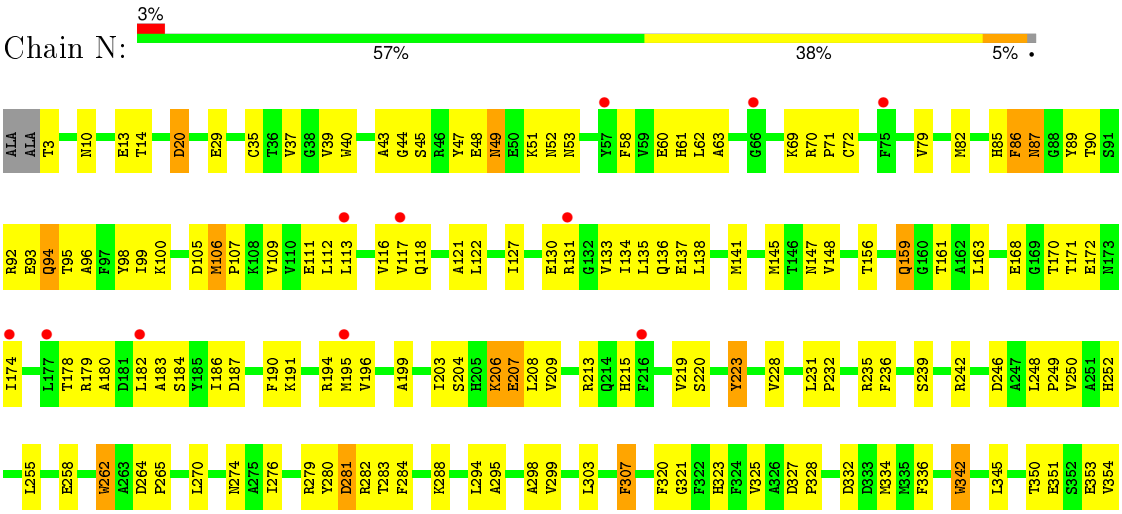
• Molecule 1: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN I

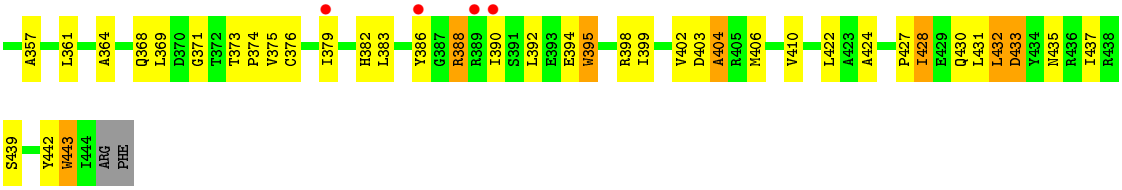
Chain A:



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

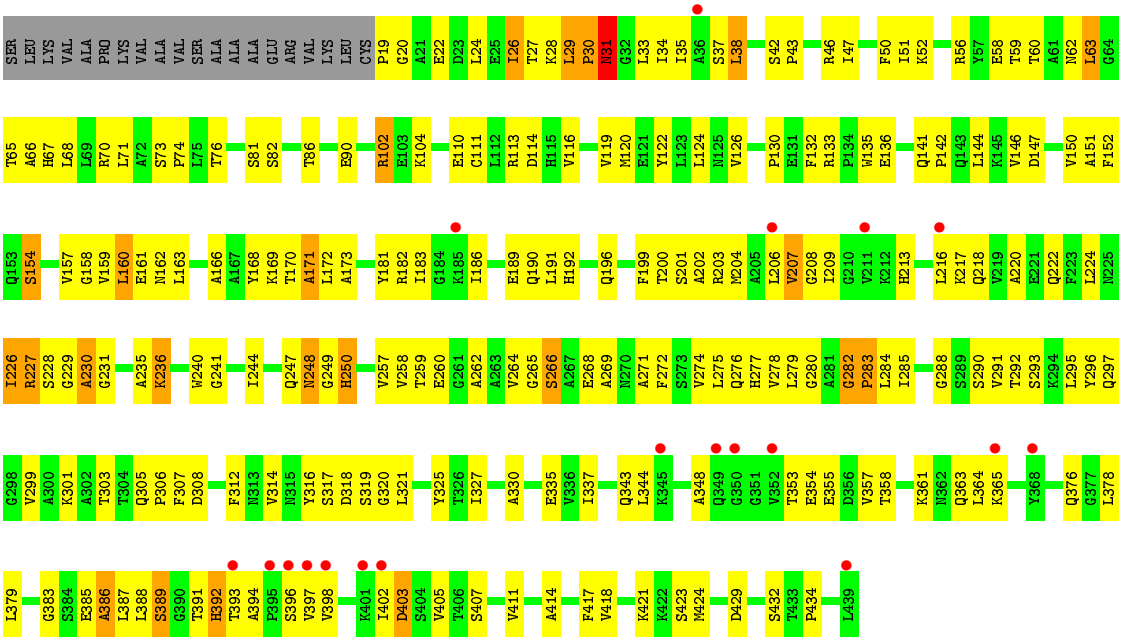
Chain N:





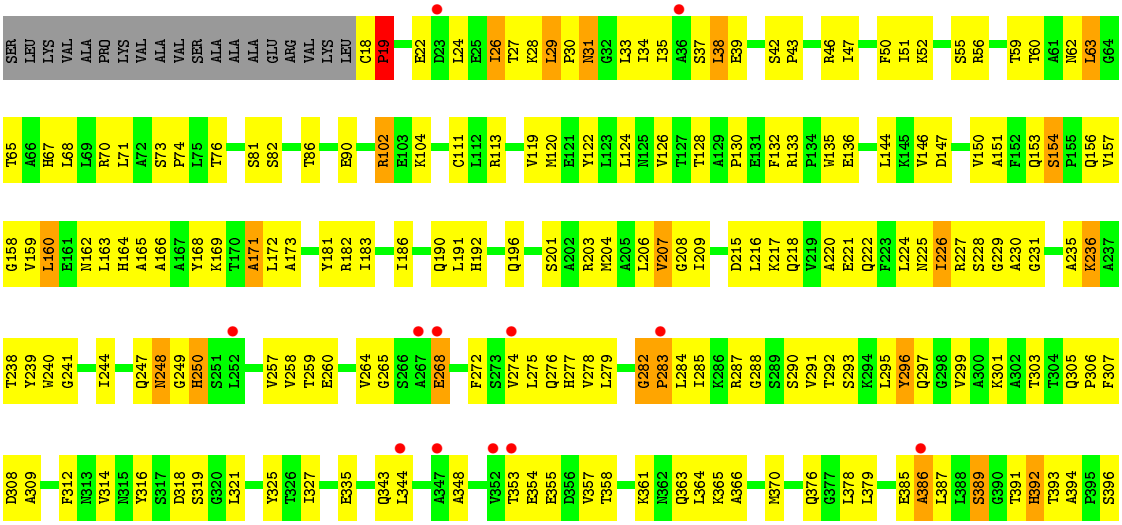
• Molecule 2: MITOCHONDRIAL UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 2

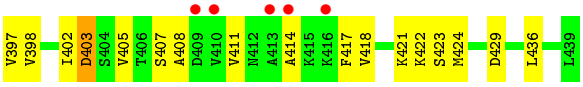
Chain B:



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

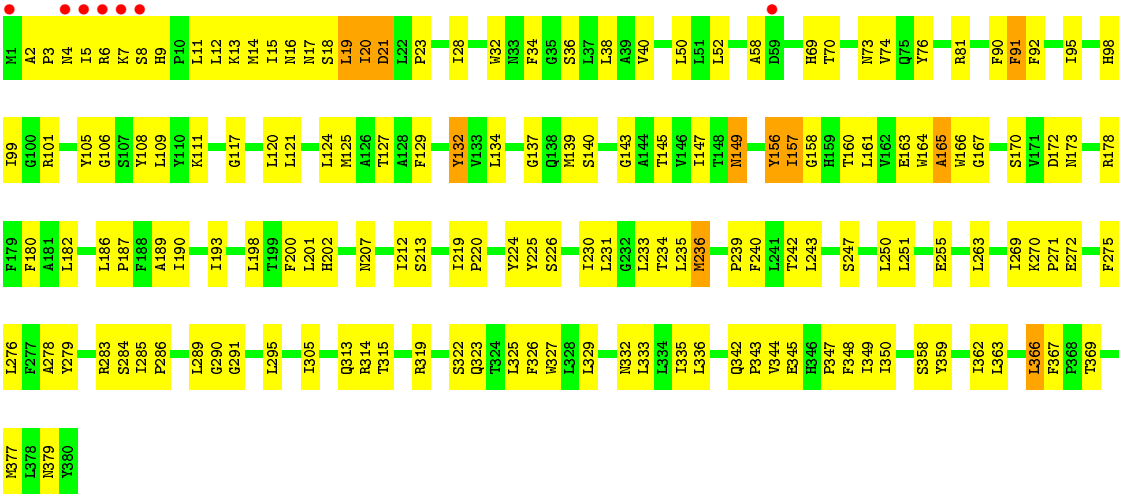
Chain O:





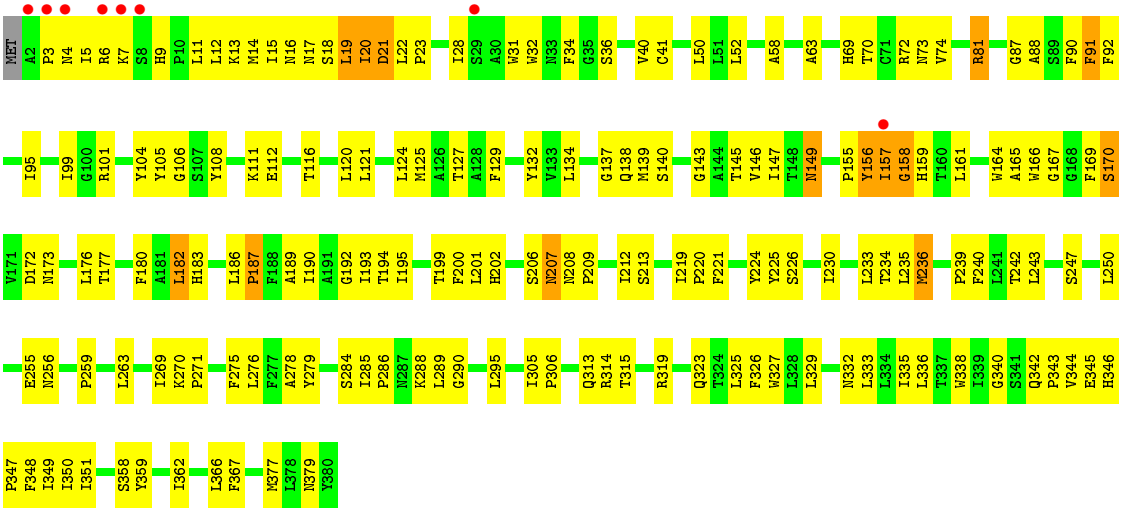
• Molecule 3: Cytochrome b

Chain C:



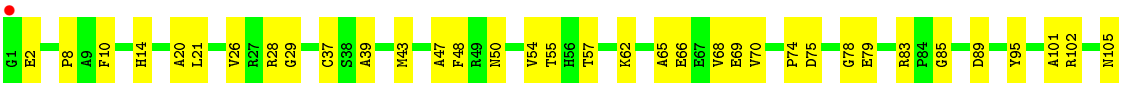
• Molecule 3: Cytochrome b

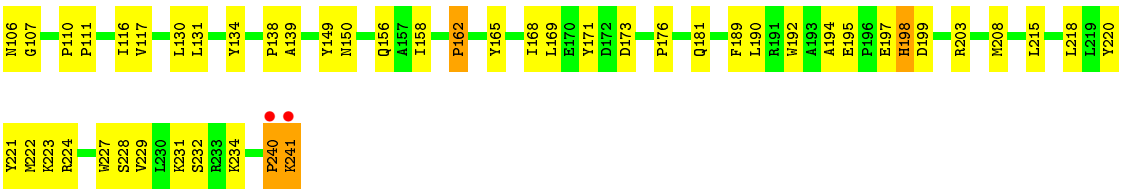
Chain P:



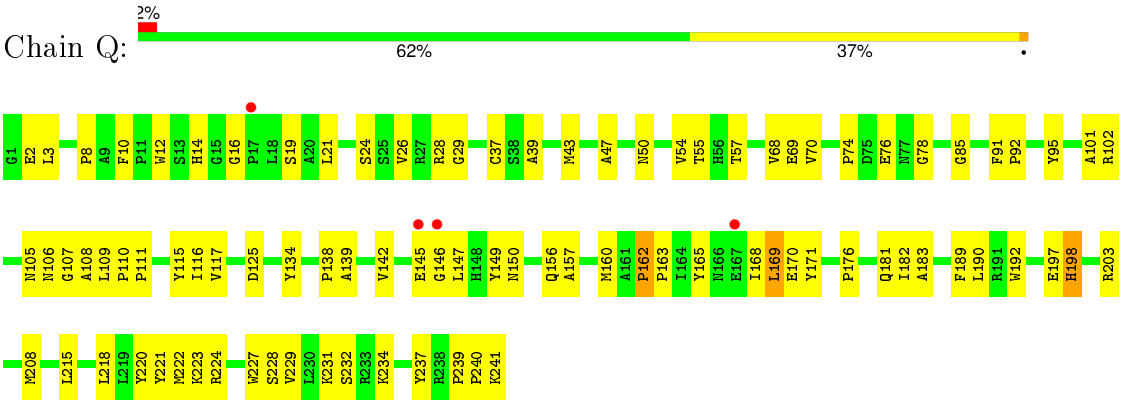
• Molecule 4: MITOCHONDRIAL CYTOCHROME C1, HEME PROTEIN

Chain D:

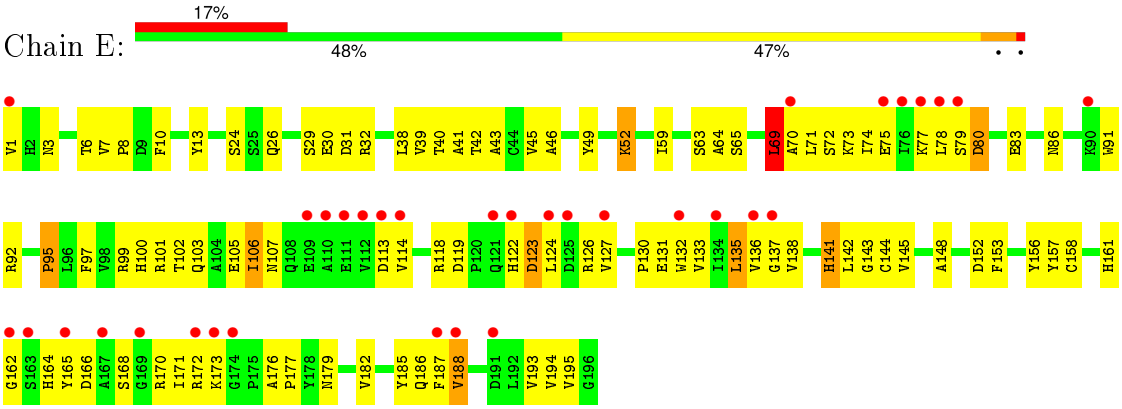




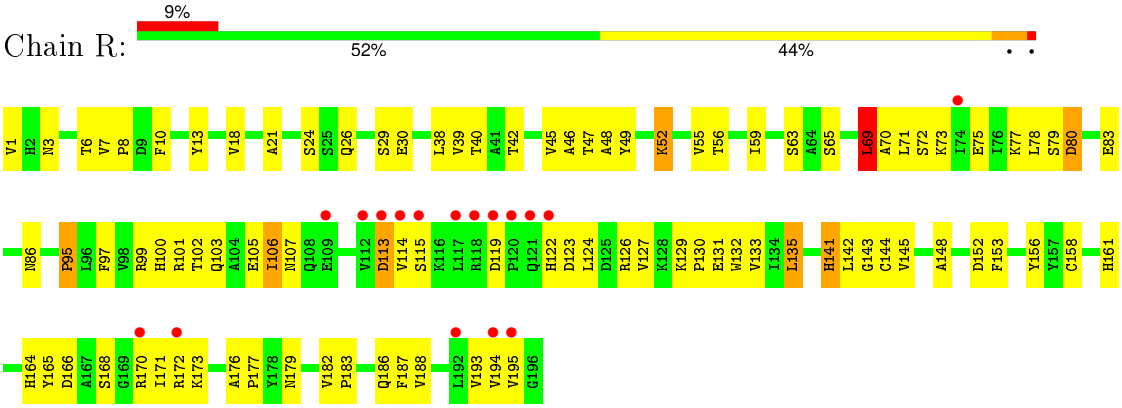
• Molecule 4: MITOCHONDRIAL CYTOCHROME C1, HEME PROTEIN



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

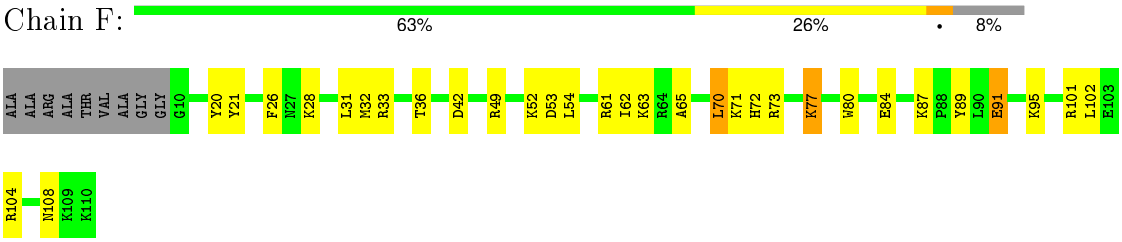


• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial



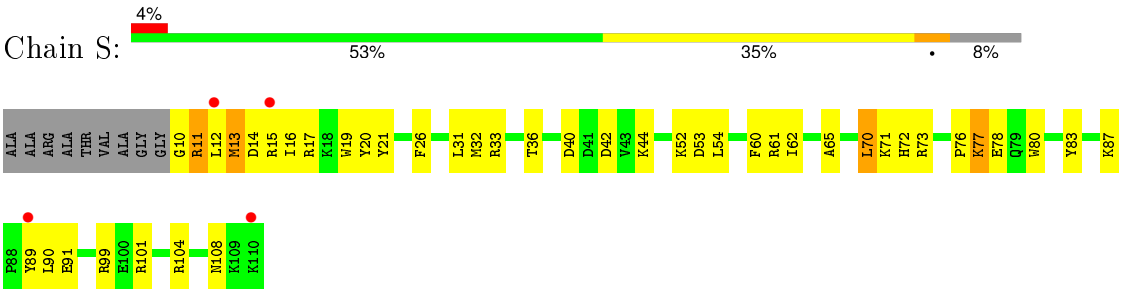
• Molecule 6: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 14 KDA PROTEIN

Chain F:



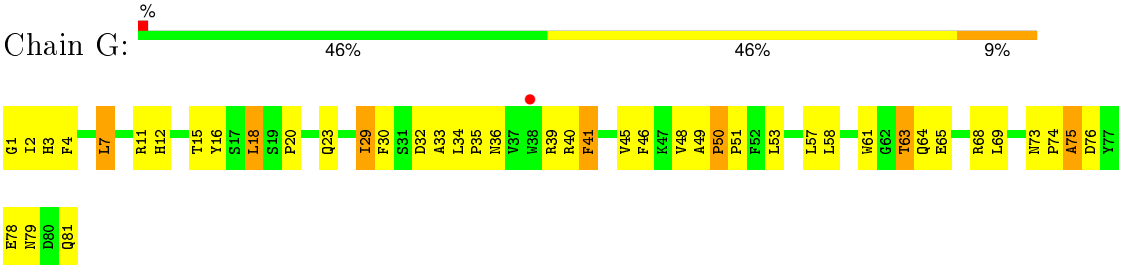
• Molecule 6: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 14 KDA PROTEIN

Chain S:



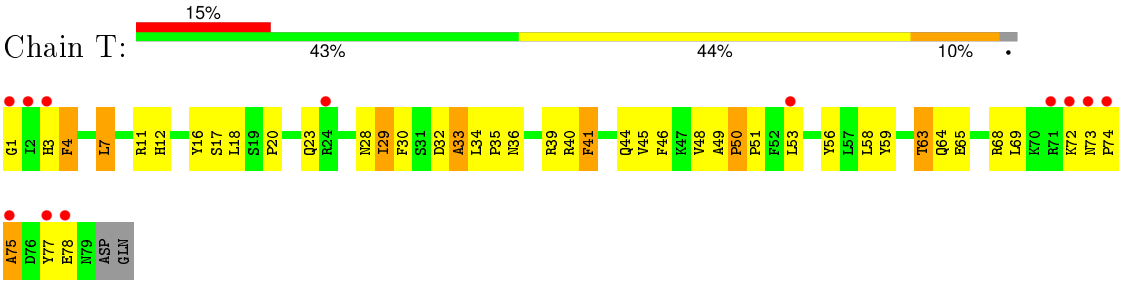
• Molecule 7: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE UBIQUINONE-BINDING PROTEIN QP-C

Chain G:



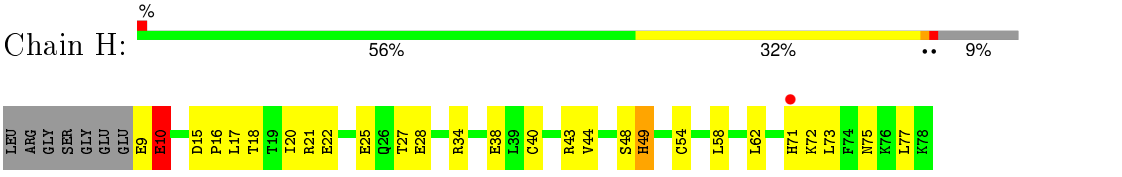
• Molecule 7: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE UBIQUINONE-BINDING PROTEIN QP-C

Chain T:



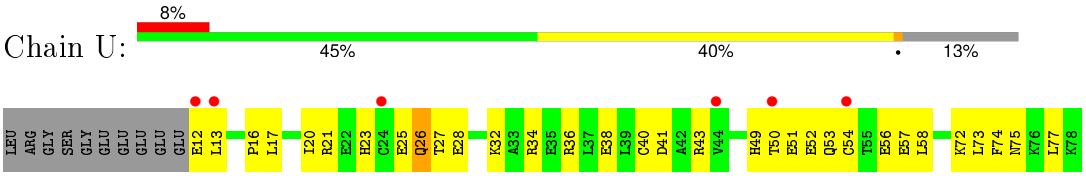
• Molecule 8: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 11 KDA PROTEIN, COMPLEX III SUBUNIT VIII

Chain H:



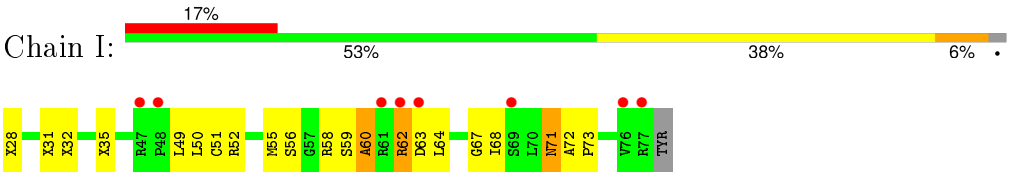
• Molecule 8: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 11 KDA PROTEIN, COMPLEX III SUBUNIT VIII

Chain U:



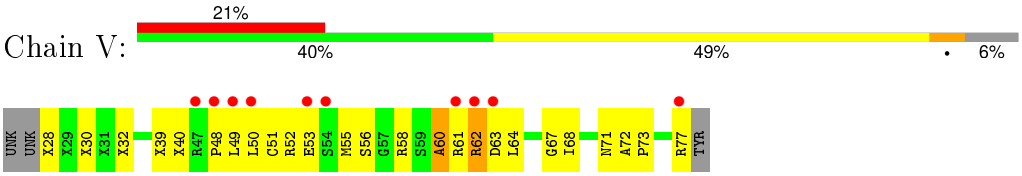
• Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain I:



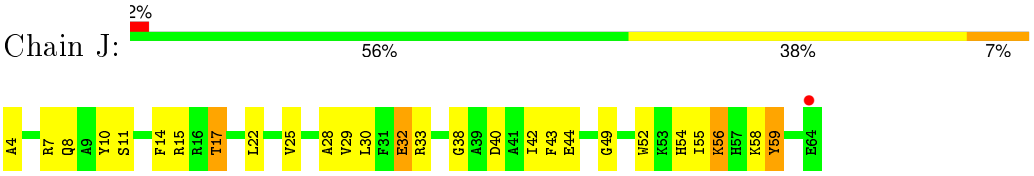
• Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial

Chain V:



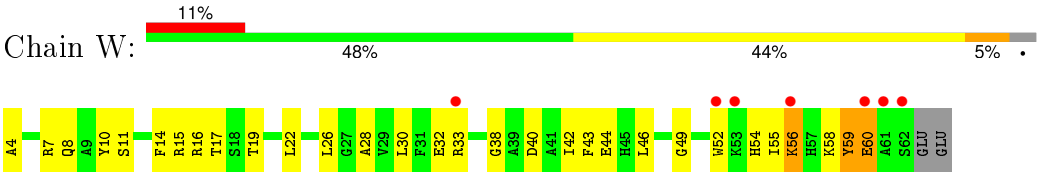
• Molecule 10: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 7.2 KDA PROTEIN

Chain J:



• Molecule 10: MITOCHONDRIAL UBIQUINOL-CYTOCHROME C REDUCTASE 7.2 KDA PROTEIN

Chain W:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	174.14Å 182.36Å 241.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.99 – 3.21 39.96 – 3.21	Depositor EDS
% Data completeness (in resolution range)	99.1 (29.99-3.21) 99.2 (39.96-3.21)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$< I/\sigma(I) >$ [1]	1.98 (at 3.18Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.267 , 0.295 0.254 , 0.283	Depositor DCC
R_{free} test set	2489 reflections (2.03%)	DCC
Wilson B-factor (Å^2)	92.9	Xtriage
Anisotropy	0.613	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 56.5	EDS
Estimated twinning fraction	0.006 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 125230 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	32657	wwPDB-VP
Average B, all atoms (Å^2)	105.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.76% 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, 3H1, CDL, FES, HEC, PEE, UNL, 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	0/3511	0.65	0/4757
1	N	0.45	0/3508	0.67	0/4753
2	B	0.39	0/3196	0.65	0/4334
2	O	0.43	0/3202	0.65	0/4343
3	C	0.59	2/3122 (0.1%)	0.73	0/4273
3	P	0.50	0/3114	0.69	0/4263
4	D	0.50	0/1956	0.68	0/2658
4	Q	0.40	0/1956	0.62	0/2658
5	E	0.39	0/1547	0.66	1/2103 (0.0%)
5	R	0.41	0/1547	0.68	1/2103 (0.0%)
6	F	0.56	0/911	0.73	0/1218
6	S	0.43	0/911	0.65	0/1218
7	G	0.57	0/698	0.72	1/946 (0.1%)
7	T	0.43	0/680	0.68	1/923 (0.1%)
8	H	0.49	0/582	0.61	0/779
8	U	0.37	0/561	0.56	0/751
9	I	0.40	0/218	0.63	0/293
9	V	0.41	0/218	0.66	0/293
10	J	0.43	0/508	0.63	0/682
10	W	0.41	0/489	0.62	0/658
All	All	0.46	2/32435 (0.0%)	0.67	4/44006 (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
3	C	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	132	TYR	CD1-CE1	5.29	1.47	1.39
3	C	132	TYR	CD2-CE2	5.08	1.47	1.39

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	143	GLY	N-CA-C	6.38	129.05	113.10
5	R	143	GLY	N-CA-C	6.27	128.77	113.10
7	T	18	LEU	CA-CB-CG	5.87	128.80	115.30
7	G	18	LEU	CA-CB-CG	5.68	128.37	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	76	TYR	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3440	0	3353	173	0
1	N	3437	0	3349	166	0
2	B	3141	0	3142	212	0
2	O	3147	0	3146	205	0
3	C	3020	0	3070	158	0
3	P	3012	0	3058	174	0
4	D	1898	0	1846	69	0
4	Q	1898	0	1846	86	0
5	E	1513	0	1478	81	0
5	R	1513	0	1478	79	0
6	F	891	0	900	36	0
6	S	891	0	900	37	0
7	G	676	0	659	48	0
7	T	658	0	647	54	0
8	H	574	0	548	23	0
8	U	553	0	535	37	0
9	I	285	0	239	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	V	275	0	238	33	0
10	J	497	0	490	21	0
10	W	478	0	478	30	0
11	A	21	0	13	0	0
11	C	49	0	72	0	0
11	E	50	0	77	0	0
11	P	54	0	72	3	0
11	R	50	0	77	3	0
12	A	1	0	0	0	0
12	C	4	0	0	1	0
12	E	1	0	0	0	0
12	P	5	0	0	0	0
12	R	1	0	0	0	0
13	C	86	0	60	12	0
13	P	86	0	60	7	0
14	C	56	0	56	3	0
14	P	56	0	58	9	0
15	C	50	0	44	2	0
15	G	40	0	24	1	0
15	P	50	0	44	1	0
15	T	40	0	24	1	0
16	C	6	0	8	0	0
16	P	6	0	8	0	0
17	D	43	0	30	3	0
17	Q	43	0	30	3	0
18	D	20	0	28	1	0
18	R	20	0	28	1	0
19	E	4	0	0	1	0
19	R	4	0	0	1	0
20	B	1	0	0	0	0
20	C	6	0	0	1	0
20	P	6	0	0	1	0
20	U	1	0	0	0	0
All	All	32657	0	32213	1589	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 24.

All (1589) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:157:VAL:HG23	9:V:64:LEU:HD21	1.15	1.13
2:O:206:LEU:HD23	2:O:220:ALA:HB2	1.40	0.99
3:P:139:MET:HE1	3:P:269:ILE:HA	1.39	0.99
6:F:52:LYS:HZ1	7:G:11:ARG:HH11	0.95	0.95
3:C:13:LYS:O	3:C:17:ASN:HB2	1.66	0.95
4:D:47:ALA:H	4:D:50:ASN:HD22	1.09	0.94
3:C:139:MET:HE1	3:C:269:ILE:HA	1.49	0.93
2:B:157:VAL:HG23	9:I:64:LEU:HD21	1.50	0.93
4:Q:47:ALA:H	4:Q:50:ASN:HD22	1.08	0.93
4:Q:231:LYS:O	6:S:71:LYS:HE3	1.69	0.93
2:O:76:THR:HG22	2:O:82:SER:H	1.31	0.92
2:O:353:THR:HG22	2:O:355:GLU:H	1.32	0.92
6:S:52:LYS:HZ1	7:T:11:ARG:NH1	1.67	0.92
2:B:76:THR:HG22	2:B:82:SER:H	1.32	0.91
6:S:52:LYS:NZ	7:T:11:ARG:HH11	1.69	0.91
5:E:97:PHE:HB2	5:E:135:LEU:HD12	1.51	0.91
3:P:13:LYS:O	3:P:17:ASN:HB2	1.69	0.90
3:P:19:LEU:O	3:P:20:ILE:HG13	1.71	0.90
3:C:129:PHE:CE1	3:C:147:ILE:HD12	2.06	0.90
6:F:52:LYS:HZ1	7:G:11:ARG:NH1	1.71	0.89
3:C:19:LEU:O	3:C:20:ILE:HG13	1.73	0.88
3:P:157:ILE:HG13	3:P:158:GLY:H	1.39	0.88
2:B:227:ARG:HD3	2:B:228:SER:H	1.38	0.88
2:O:128:THR:HA	2:O:226:ILE:HD11	1.54	0.88
4:Q:74:PRO:HB2	4:Q:78:GLY:HA2	1.56	0.87
6:F:32:MET:CE	6:F:87:LYS:HG2	2.04	0.87
6:S:52:LYS:HZ1	7:T:11:ARG:HH11	0.90	0.87
5:R:97:PHE:HB2	5:R:135:LEU:HD12	1.56	0.86
9:I:32:UNK:N	9:I:73:PRO:HG2	1.90	0.86
2:B:353:THR:HG22	2:B:355:GLU:H	1.39	0.86
2:B:218:GLN:HG3	2:B:222:GLN:HE22	1.39	0.86
1:A:170:THR:HG22	1:A:171:THR:H	1.40	0.86
1:N:390:ILE:HG23	1:N:394:GLU:OE1	1.76	0.86
2:B:199:PHE:O	2:B:226:ILE:HG12	1.74	0.85
1:N:231:LEU:HD23	1:N:232:PRO:HD2	1.58	0.85
3:P:127:THR:HG21	13:P:501:HEM:HBB2	1.55	0.85
6:F:52:LYS:NZ	7:G:11:ARG:HH11	1.74	0.85
9:I:71:ASN:HD22	9:I:71:ASN:H	1.25	0.85
2:B:227:ARG:NE	2:B:227:ARG:HA	1.91	0.84
2:B:283:PRO:HG3	9:I:56:SER:HB2	1.58	0.84
4:D:74:PRO:HB2	4:D:78:GLY:HA2	1.59	0.84
2:B:207:VAL:HG12	2:B:208:GLY:H	1.43	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:220:ALA:O	2:O:224:LEU:HB2	1.77	0.84
2:O:27:THR:HG22	2:O:28:LYS:H	1.42	0.84
2:O:221:GLU:HG3	2:O:222:GLN:H	1.42	0.83
1:N:170:THR:HG22	1:N:171:THR:H	1.40	0.83
3:P:50:LEU:HD23	13:P:501:HEM:HBC1	1.60	0.83
2:O:22:GLU:HG3	2:O:39:GLU:HB3	1.60	0.83
1:A:390:ILE:HG23	1:A:394:GLU:OE1	1.77	0.83
5:R:1:VAL:HG23	5:R:3:ASN:H	1.44	0.83
1:N:136:GLN:NE2	9:V:50:LEU:HB2	1.94	0.82
1:N:105:ASP:O	1:N:109:VAL:HG23	1.78	0.82
1:A:364:ALA:O	1:A:368:GLN:HG2	1.79	0.82
2:B:227:ARG:HE	2:B:227:ARG:HA	1.45	0.82
2:O:76:THR:CG2	2:O:82:SER:H	1.93	0.81
2:B:203:ARG:HD2	2:B:230:ALA:HA	1.62	0.81
3:C:127:THR:HG21	13:C:501:HEM:HBB2	1.60	0.81
3:P:325:LEU:HD21	3:P:366:LEU:HB3	1.60	0.81
3:P:15:ILE:H	3:P:15:ILE:HD12	1.45	0.81
1:N:49:ASN:ND2	1:N:52:ASN:H	1.79	0.81
3:C:6:ARG:HD3	3:C:16:ASN:OD1	1.81	0.81
3:C:15:ILE:HD12	3:C:15:ILE:H	1.45	0.81
3:P:17:ASN:HD21	7:T:1:GLY:HA2	1.46	0.81
1:A:170:THR:HG22	1:A:171:THR:N	1.96	0.81
2:O:285:ILE:HG13	2:O:288:GLY:HA3	1.63	0.81
2:B:76:THR:CG2	2:B:82:SER:H	1.94	0.80
3:C:2:ALA:HB3	3:C:8:SER:HB3	1.63	0.80
8:U:73:LEU:HD12	8:U:73:LEU:O	1.82	0.80
4:Q:139:ALA:HB3	8:U:54:CYS:SG	2.21	0.80
2:O:130:PRO:HB2	2:O:132:PHE:CE2	2.17	0.80
4:D:231:LYS:O	6:F:71:LYS:HE3	1.81	0.80
3:C:342:GLN:HA	3:C:342:GLN:HE21	1.44	0.79
1:A:197:LEU:HD22	1:A:216:PHE:HE1	1.47	0.79
1:N:388:ARG:HH21	1:N:388:ARG:HG3	1.48	0.79
2:O:62:ASN:O	2:O:65:THR:HG22	1.83	0.79
2:O:27:THR:HG22	2:O:28:LYS:N	1.98	0.79
4:D:222:MET:HE1	5:E:40:THR:HG23	1.64	0.79
4:D:241:LYS:HE3	4:D:241:LYS:HA	1.63	0.79
1:N:196:VAL:HG11	1:N:383:LEU:HD12	1.64	0.78
2:O:283:PRO:HG3	9:V:56:SER:HB2	1.65	0.78
6:F:32:MET:CE	6:F:87:LYS:H	1.97	0.78
4:Q:54:VAL:HG12	4:Q:55:THR:HG23	1.65	0.78
2:O:292:THR:HG21	2:O:363:GLN:HE22	1.48	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:130:PRO:HB2	2:B:132:PHE:CE2	2.19	0.78
1:N:170:THR:HG22	1:N:171:THR:N	1.98	0.78
3:P:6:ARG:HD3	3:P:16:ASN:OD1	1.84	0.77
6:F:32:MET:HE2	6:F:87:LYS:HG2	1.65	0.77
10:J:10:TYR:CE2	10:J:15:ARG:HD2	2.19	0.77
2:B:62:ASN:O	2:B:65:THR:HG22	1.84	0.77
2:B:63:LEU:HB2	2:B:182:ARG:HD3	1.66	0.77
2:O:157:VAL:CG2	9:V:64:LEU:HD21	2.07	0.77
2:O:226:ILE:HG22	2:O:227:ARG:N	1.99	0.77
1:N:364:ALA:O	1:N:368:GLN:HG2	1.84	0.77
1:N:37:VAL:HG12	1:N:199:ALA:HB1	1.66	0.77
1:N:443:TRP:CE3	1:N:443:TRP:HA	2.19	0.77
3:P:157:ILE:HG13	3:P:158:GLY:N	1.99	0.77
10:W:10:TYR:CE2	10:W:15:ARG:HD2	2.19	0.77
2:O:225:ASN:CG	2:O:226:ILE:H	1.88	0.76
3:C:342:GLN:HA	3:C:342:GLN:NE2	2.01	0.76
3:C:90:PHE:HB3	3:C:236:MET:HE3	1.66	0.76
2:B:285:ILE:HG13	2:B:288:GLY:HA3	1.66	0.76
13:P:501:HEM:HBC2	13:P:501:HEM:HMC1	1.67	0.76
2:O:207:VAL:HG12	2:O:208:GLY:H	1.50	0.76
4:Q:197:GLU:HG2	4:Q:198:HIS:N	1.99	0.76
1:A:373:THR:HB	1:A:374:PRO:HD3	1.67	0.76
3:C:325:LEU:HD21	3:C:366:LEU:HB3	1.66	0.76
5:E:73:LYS:HB3	5:E:195:VAL:O	1.86	0.76
2:O:102:ARG:HG2	2:O:102:ARG:HH11	1.51	0.76
2:O:226:ILE:HG22	2:O:227:ARG:H	1.50	0.75
2:B:201:SER:OG	2:B:228:SER:HB3	1.87	0.75
2:O:63:LEU:HB2	2:O:182:ARG:HD3	1.67	0.75
1:A:49:ASN:ND2	1:A:52:ASN:H	1.85	0.75
3:C:17:ASN:HD21	7:G:1:GLY:HA2	1.52	0.75
1:N:206:LYS:O	1:N:209:VAL:HG12	1.87	0.74
1:N:182:LEU:O	1:N:186:ILE:HG13	1.87	0.74
8:U:40:CYS:HA	8:U:43:ARG:NH1	2.01	0.74
4:Q:229:VAL:HG23	7:T:20:PRO:HG3	1.69	0.74
4:D:54:VAL:HG12	4:D:55:THR:HG23	1.69	0.74
1:A:131:ARG:HG3	1:A:131:ARG:HH11	1.50	0.74
5:R:75:GLU:HG2	5:R:194:VAL:HG22	1.70	0.74
6:S:52:LYS:NZ	7:T:11:ARG:NH1	2.31	0.74
1:N:136:GLN:HE22	9:V:50:LEU:HD12	1.51	0.74
2:O:29:LEU:HD11	2:O:221:GLU:HB3	1.70	0.73
2:B:306:PRO:HA	9:I:52:ARG:HG3	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:292:THR:HG21	2:B:363:GLN:HE22	1.53	0.73
1:A:182:LEU:O	1:A:186:ILE:HG13	1.89	0.73
3:P:129:PHE:CE1	3:P:147:ILE:HD12	2.24	0.73
3:P:12:LEU:HA	3:P:15:ILE:HD13	1.71	0.73
1:A:196:VAL:HG11	1:A:383:LEU:HD12	1.70	0.73
4:Q:8:PRO:HG2	4:Q:10:PHE:CE1	2.24	0.73
1:A:85:HIS:HB2	1:A:100:LYS:HB2	1.70	0.73
2:B:209:ILE:HD13	2:B:378:LEU:HD23	1.70	0.73
3:P:70:THR:O	3:P:74:VAL:HB	1.89	0.72
1:A:388:ARG:HG3	1:A:388:ARG:HH21	1.53	0.72
5:E:75:GLU:HG2	5:E:194:VAL:HG22	1.71	0.72
5:R:186:GLN:HE21	5:R:188:VAL:HG12	1.55	0.72
2:O:295:LEU:O	2:O:299:VAL:HG23	1.90	0.72
7:T:29:ILE:HD12	7:T:29:ILE:H	1.55	0.72
7:G:50:PRO:HB2	7:G:51:PRO:CD	2.20	0.72
6:F:52:LYS:NZ	7:G:11:ARG:NH1	2.36	0.72
2:O:398:VAL:O	2:O:402:ILE:HG13	1.90	0.72
17:D:501:HEC:HBB3	17:D:501:HEC:HMB1	1.71	0.72
4:Q:223:LYS:C	4:Q:223:LYS:HD3	2.10	0.72
3:C:12:LEU:HA	3:C:15:ILE:HD13	1.72	0.71
5:R:131:GLU:HG2	5:R:132:TRP:CD1	2.24	0.71
6:F:32:MET:HE3	6:F:87:LYS:HG2	1.73	0.71
2:O:133:ARG:HD3	2:O:135:TRP:CZ2	2.25	0.71
1:N:49:ASN:HD21	1:N:52:ASN:H	1.39	0.71
3:P:101:ARG:C	3:P:101:ARG:HD2	2.11	0.71
2:O:29:LEU:HB3	2:O:30:PRO:HD2	1.71	0.71
7:T:50:PRO:HB2	7:T:51:PRO:CD	2.21	0.71
4:Q:47:ALA:N	4:Q:50:ASN:HD22	1.88	0.71
9:I:71:ASN:N	9:I:71:ASN:HD22	1.87	0.71
5:E:1:VAL:HG23	5:E:3:ASN:H	1.56	0.71
8:U:52:GLU:HG2	8:U:53:GLN:N	2.06	0.70
2:B:295:LEU:O	2:B:299:VAL:HG23	1.90	0.70
1:N:443:TRP:HE3	1:N:443:TRP:HA	1.53	0.70
2:O:393:THR:HG23	2:O:397:VAL:HB	1.74	0.70
2:B:29:LEU:HB3	2:B:30:PRO:HD2	1.71	0.70
3:P:347:PRO:O	3:P:350:ILE:HG22	1.90	0.70
2:O:47:ILE:HD12	2:O:47:ILE:N	2.06	0.70
1:A:369:LEU:HD11	1:A:392:LEU:HD21	1.72	0.70
1:N:131:ARG:HG3	1:N:131:ARG:HH11	1.57	0.70
4:D:197:GLU:HG2	4:D:198:HIS:N	2.07	0.70
2:B:393:THR:HG23	2:B:397:VAL:HB	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:33:LEU:HD21	2:B:224:LEU:HD12	1.74	0.70
2:B:393:THR:CG2	2:B:397:VAL:HB	2.21	0.70
1:N:373:THR:HB	1:N:374:PRO:HD3	1.71	0.70
2:O:292:THR:HG21	2:O:363:GLN:NE2	2.07	0.69
1:N:37:VAL:HG12	1:N:199:ALA:CB	2.22	0.69
4:D:181:GLN:HA	8:H:77:LEU:HD22	1.74	0.69
1:A:37:VAL:HG12	1:A:199:ALA:HB1	1.74	0.69
1:A:233:ARG:HG2	1:A:233:ARG:HH11	1.58	0.69
2:B:206:LEU:HG	2:B:216:LEU:HD11	1.73	0.69
1:A:186:ILE:HG23	1:A:190:PHE:CD1	2.27	0.69
3:P:285:ILE:HD12	3:P:285:ILE:N	2.08	0.69
3:P:342:GLN:HE21	3:P:342:GLN:HA	1.57	0.69
1:A:443:TRP:CE3	1:A:443:TRP:HA	2.28	0.69
4:D:223:LYS:HD3	4:D:223:LYS:C	2.13	0.69
2:O:376:GLN:HE22	9:V:77:ARG:HH22	1.40	0.69
3:C:285:ILE:N	3:C:285:ILE:HD12	2.07	0.69
3:P:235:LEU:O	3:P:239:PRO:HD2	1.93	0.68
3:P:342:GLN:HE21	3:P:343:PRO:HD2	1.58	0.68
2:O:225:ASN:CG	2:O:226:ILE:N	2.43	0.68
2:B:47:ILE:HG12	2:B:120:MET:HE3	1.74	0.68
2:B:132:PHE:CD1	2:B:191:LEU:HB3	2.29	0.68
3:C:69:HIS:CD2	3:C:73:ASN:HD22	2.12	0.68
2:O:357:VAL:O	2:O:361:LYS:HG3	1.93	0.68
2:O:227:ARG:NH1	2:O:228:SER:H	1.92	0.68
3:C:139:MET:SD	3:C:269:ILE:HG13	2.34	0.68
1:A:197:LEU:HD22	1:A:216:PHE:CE1	2.26	0.68
2:B:47:ILE:N	2:B:47:ILE:HD12	2.09	0.68
2:B:357:VAL:O	2:B:361:LYS:HG3	1.94	0.68
2:B:102:ARG:HG2	2:B:102:ARG:HH11	1.59	0.68
3:P:17:ASN:HD21	7:T:1:GLY:CA	2.07	0.68
4:D:149:TYR:CE1	4:D:156:GLN:HB3	2.29	0.68
2:B:398:VAL:O	2:B:402:ILE:HG13	1.94	0.67
6:F:32:MET:HE3	6:F:87:LYS:H	1.58	0.67
3:C:15:ILE:HD12	3:C:15:ILE:N	2.08	0.67
2:O:393:THR:CG2	2:O:397:VAL:HB	2.24	0.67
1:N:342:TRP:O	1:N:345:LEU:HB2	1.93	0.67
2:O:34:ILE:HD13	2:O:386:ALA:O	1.94	0.67
3:C:2:ALA:CB	3:C:8:SER:HB3	2.24	0.67
2:B:248:ASN:HD22	2:B:248:ASN:C	1.98	0.67
1:N:85:HIS:HB2	1:N:100:LYS:HB2	1.75	0.67
4:Q:76:GLU:CD	4:Q:76:GLU:H	1.98	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:34:ARG:O	8:U:38:GLU:HG2	1.94	0.67
1:A:231:LEU:HD23	1:A:232:PRO:HD2	1.76	0.67
8:H:73:LEU:HD12	8:H:73:LEU:O	1.95	0.67
5:E:131:GLU:HG2	5:E:132:TRP:CD1	2.30	0.67
2:B:24:LEU:HD12	2:B:37:SER:O	1.95	0.67
5:R:45:VAL:HG13	10:W:28:ALA:HA	1.77	0.67
2:O:248:ASN:HD22	2:O:248:ASN:C	1.96	0.67
5:E:97:PHE:HB2	5:E:135:LEU:CD1	2.24	0.67
2:O:59:THR:HG22	2:O:60:THR:N	2.08	0.67
3:P:17:ASN:ND2	7:T:1:GLY:HA2	2.10	0.66
1:N:395:TRP:HA	1:N:395:TRP:CE3	2.28	0.66
5:R:30:GLU:HB2	10:W:7:ARG:HG2	1.77	0.66
1:N:369:LEU:HD11	1:N:392:LEU:HD21	1.77	0.66
3:C:342:GLN:HE21	3:C:343:PRO:HD2	1.60	0.66
2:O:51:ILE:HG12	2:O:204:MET:HG2	1.75	0.66
1:A:134:ILE:HG21	1:A:174:ILE:HD13	1.77	0.66
1:A:336:PHE:CZ	3:C:4:ASN:HB3	2.30	0.66
1:A:60:GLU:OE2	1:A:90:THR:HG22	1.95	0.66
2:B:46:ARG:NH2	2:B:376:GLN:HG3	2.10	0.66
2:B:227:ARG:CD	2:B:228:SER:H	2.08	0.66
4:Q:222:MET:HE3	5:R:40:THR:HG23	1.76	0.66
2:B:325:TYR:CD1	9:I:60:ALA:HB2	2.31	0.66
3:P:236:MET:HA	15:P:3003:CDL:H162	1.78	0.66
4:D:47:ALA:N	4:D:50:ASN:HD22	1.90	0.66
1:A:170:THR:CG2	1:A:171:THR:H	2.09	0.66
2:B:51:ILE:HG12	2:B:204:MET:HG2	1.77	0.66
1:N:60:GLU:OE2	1:N:90:THR:HG22	1.95	0.66
3:P:15:ILE:N	3:P:15:ILE:HD12	2.11	0.65
1:A:137:GLU:O	1:A:141:MET:HG3	1.94	0.65
1:A:49:ASN:HD21	1:A:52:ASN:H	1.42	0.65
10:J:4:ALA:O	10:J:8:GLN:HG3	1.95	0.65
3:P:92:PHE:O	3:P:95:ILE:HG22	1.96	0.65
5:E:99:ARG:HB3	5:E:133:VAL:CG1	2.26	0.65
4:D:26:VAL:HG12	4:D:55:THR:HG21	1.78	0.65
10:W:52:TRP:O	10:W:56:LYS:HB2	1.96	0.65
5:R:73:LYS:HB3	5:R:195:VAL:O	1.96	0.65
1:N:10:ASN:ND2	2:O:19:PRO:HB2	2.12	0.65
4:Q:237:TYR:HB2	6:S:60:PHE:CD1	2.31	0.65
17:Q:501:HEC:HMB1	17:Q:501:HEC:HBB3	1.79	0.65
3:C:101:ARG:C	3:C:101:ARG:HD2	2.16	0.65
3:P:269:ILE:HG23	3:P:269:ILE:O	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:50:LEU:HD23	13:C:501:HEM:HBC1	1.78	0.65
2:O:389:SER:O	2:O:391:THR:HG23	1.97	0.65
3:P:120:LEU:HD22	13:P:502:HEM:CBB	2.26	0.65
7:G:78:GLU:C	7:G:79:ASN:HD22	2.00	0.65
2:O:144:LEU:HB2	2:O:183:ILE:HD12	1.78	0.65
1:A:37:VAL:HG23	1:A:113:LEU:HD11	1.78	0.65
1:N:49:ASN:C	1:N:49:ASN:ND2	2.48	0.65
4:D:29:GLY:HA3	4:D:189:PHE:HB2	1.79	0.65
2:B:292:THR:HG21	2:B:363:GLN:NE2	2.11	0.64
1:A:395:TRP:HA	1:A:395:TRP:CE3	2.32	0.64
1:N:37:VAL:HG23	1:N:113:LEU:HD11	1.79	0.64
2:B:27:THR:HG22	2:B:28:LYS:N	2.12	0.64
1:A:443:TRP:HE3	1:A:443:TRP:HA	1.62	0.64
17:Q:501:HEC:HBA1	17:Q:501:HEC:HHA	1.79	0.64
3:P:69:HIS:CD2	3:P:73:ASN:HD22	2.16	0.64
2:B:218:GLN:HG3	2:B:222:GLN:NE2	2.10	0.64
3:C:305:ILE:HD11	3:C:363:LEU:HD22	1.80	0.64
4:D:229:VAL:HG23	7:G:20:PRO:HG3	1.79	0.64
1:N:44:GLY:H	1:N:47:TYR:HD1	1.44	0.64
7:T:3:HIS:O	7:T:7:LEU:HG	1.97	0.64
5:R:97:PHE:HB2	5:R:135:LEU:CD1	2.26	0.64
4:D:116:ILE:HG21	4:D:190:LEU:HD13	1.80	0.64
3:C:235:LEU:O	3:C:239:PRO:HD2	1.97	0.64
1:A:35:CYS:SG	1:A:203:ILE:HD11	2.38	0.64
3:C:120:LEU:HD22	13:C:502:HEM:CBB	2.28	0.64
1:A:49:ASN:ND2	1:A:49:ASN:C	2.48	0.64
2:B:389:SER:O	2:B:391:THR:HG23	1.97	0.64
2:O:226:ILE:CG2	2:O:227:ARG:H	2.11	0.64
2:B:162:ASN:O	2:B:244:ILE:HD12	1.98	0.64
3:P:157:ILE:CG1	3:P:158:GLY:H	2.09	0.64
4:Q:237:TYR:HB2	6:S:60:PHE:CG	2.33	0.64
1:N:161:THR:HG21	1:N:235:ARG:H	1.63	0.64
6:S:77:LYS:HA	6:S:80:TRP:CE2	2.33	0.63
10:W:49:GLY:N	10:W:54:HIS:ND1	2.46	0.63
2:O:50:PHE:HD2	2:O:104:LYS:HZ1	1.46	0.63
1:A:105:ASP:O	1:A:109:VAL:HG23	1.98	0.63
5:E:99:ARG:HB3	5:E:133:VAL:HG13	1.80	0.63
8:H:34:ARG:O	8:H:38:GLU:HG2	1.98	0.63
2:B:297:GLN:O	2:B:301:LYS:HG3	1.97	0.63
4:Q:47:ALA:H	4:Q:50:ASN:ND2	1.89	0.63
2:B:59:THR:HG22	2:B:60:THR:N	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:314:VAL:HG13	9:V:63:ASP:HB3	1.80	0.63
2:B:264:VAL:HG11	2:B:388:LEU:HD13	1.80	0.63
1:N:223:TYR:HD2	1:N:223:TYR:H	1.45	0.63
2:O:225:ASN:ND2	2:O:226:ILE:H	1.95	0.63
3:P:106:GLY:HA2	3:P:108:TYR:CE2	2.34	0.63
4:Q:116:ILE:HG23	4:Q:117:VAL:N	2.13	0.63
1:A:223:TYR:HD2	1:A:223:TYR:H	1.44	0.63
2:O:27:THR:CG2	2:O:28:LYS:H	2.11	0.63
2:O:132:PHE:CD1	2:O:191:LEU:HB3	2.34	0.63
10:J:52:TRP:O	10:J:56:LYS:HB2	1.98	0.63
3:C:236:MET:HA	15:C:2003:CDL:H162	1.79	0.63
3:P:342:GLN:NE2	3:P:342:GLN:HA	2.14	0.63
2:O:257:VAL:HG22	2:O:424:MET:HG3	1.80	0.63
1:N:369:LEU:HD12	1:N:392:LEU:HD11	1.81	0.63
4:D:116:ILE:HG23	4:D:117:VAL:N	2.13	0.62
1:N:178:THR:HG22	1:N:179:ARG:N	2.13	0.62
2:O:209:ILE:HD13	2:O:378:LEU:HD23	1.81	0.62
1:N:49:ASN:C	1:N:49:ASN:HD22	2.01	0.62
2:B:28:LYS:O	2:B:29:LEU:O	2.17	0.62
1:A:242:ARG:HH22	1:A:432:LEU:HA	1.63	0.62
2:O:274:VAL:O	2:O:278:VAL:HG23	1.99	0.62
5:E:156:TYR:HB2	5:E:165:TYR:HB2	1.81	0.62
5:E:52:LYS:C	5:E:52:LYS:HD3	2.20	0.62
2:O:291:VAL:HA	2:O:297:GLN:HE21	1.64	0.62
3:C:347:PRO:O	3:C:350:ILE:HG22	1.99	0.62
7:T:73:ASN:HD21	7:T:75:ALA:HB3	1.65	0.62
1:N:395:TRP:HA	1:N:395:TRP:HE3	1.63	0.62
1:N:284:PHE:CE2	9:V:71:ASN:O	2.52	0.62
2:B:71:LEU:O	2:B:74:PRO:HD2	2.00	0.62
7:G:3:HIS:O	7:G:7:LEU:HG	1.99	0.62
3:P:90:PHE:CE1	3:P:240:PHE:HA	2.35	0.62
2:O:24:LEU:HD12	2:O:37:SER:O	1.98	0.62
3:C:342:GLN:HE21	3:C:342:GLN:CA	2.08	0.62
1:A:49:ASN:C	1:A:49:ASN:HD22	2.01	0.62
10:W:56:LYS:O	10:W:60:GLU:HG2	1.99	0.62
1:N:327:ASP:HB3	1:N:328:PRO:HD2	1.82	0.62
2:O:227:ARG:HH11	2:O:228:SER:H	1.47	0.62
1:N:186:ILE:HG23	1:N:190:PHE:CD1	2.35	0.62
3:P:95:ILE:O	3:P:99:ILE:HG13	2.00	0.62
4:D:240:PRO:HD3	7:G:12:HIS:CE1	2.35	0.61
1:N:170:THR:CG2	1:N:171:THR:H	2.12	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:71:LEU:O	2:O:74:PRO:HD2	2.00	0.61
3:C:92:PHE:O	3:C:95:ILE:HG22	2.00	0.61
2:O:46:ARG:NH2	2:O:376:GLN:HG3	2.16	0.61
2:O:76:THR:HG22	2:O:82:SER:N	2.10	0.61
5:E:45:VAL:HG13	10:J:28:ALA:HA	1.82	0.61
3:P:139:MET:SD	3:P:269:ILE:HG13	2.41	0.61
1:N:49:ASN:ND2	1:N:51:LYS:H	1.99	0.61
1:A:85:HIS:NE2	2:B:284:LEU:HD22	2.14	0.61
3:C:187:PRO:HG2	13:C:501:HEM:HMC1	1.82	0.61
3:C:279:TYR:O	3:C:283:ARG:HG3	2.00	0.61
1:N:106:MET:HG3	1:N:203:ILE:CG2	2.31	0.61
3:P:289:LEU:O	3:P:289:LEU:HD12	2.01	0.61
2:B:76:THR:HG22	2:B:82:SER:N	2.10	0.61
3:C:269:ILE:HG23	3:C:269:ILE:O	2.01	0.61
1:A:336:PHE:CE2	3:C:4:ASN:HB3	2.36	0.61
3:C:226:SER:O	3:C:230:ILE:HG12	2.01	0.61
3:P:219:ILE:HD12	3:P:224:TYR:CD1	2.35	0.61
1:N:45:SER:HA	1:N:48:GLU:HG3	1.82	0.61
3:C:17:ASN:HD21	7:G:1:GLY:CA	2.13	0.61
3:C:15:ILE:CD1	3:C:15:ILE:H	2.14	0.61
4:Q:54:VAL:HG11	4:Q:192:TRP:NE1	2.16	0.61
4:Q:197:GLU:HG2	4:Q:198:HIS:H	1.64	0.61
2:B:47:ILE:HG12	2:B:120:MET:CE	2.30	0.60
2:O:361:LYS:O	2:O:365:LYS:HG3	2.00	0.60
3:P:332:ASN:HD21	3:P:358:SER:CB	2.13	0.60
2:O:259:THR:HG22	2:O:260:GLU:N	2.16	0.60
2:B:35:ILE:O	2:B:213:HIS:HE1	1.85	0.60
4:D:47:ALA:H	4:D:50:ASN:ND2	1.92	0.60
2:B:264:VAL:HG23	2:B:316:TYR:C	2.21	0.60
3:P:332:ASN:ND2	3:P:358:SER:OG	2.35	0.60
1:A:19:LEU:HB2	1:A:21:ASN:OD1	2.01	0.60
2:O:277:HIS:NE2	2:O:364:LEU:HD13	2.17	0.60
6:F:61:ARG:NH2	6:F:89:TYR:CE2	2.70	0.60
9:V:64:LEU:HD12	9:V:77:ARG:O	2.02	0.60
6:S:11:ARG:HG2	6:S:11:ARG:O	2.01	0.60
1:N:35:CYS:SG	1:N:203:ILE:HD11	2.42	0.60
10:W:4:ALA:O	10:W:8:GLN:HG3	2.01	0.60
4:Q:221:TYR:CD2	5:R:39:VAL:HG11	2.37	0.60
9:V:28:UNK:CB	9:V:72:ALA:HB2	2.32	0.60
3:P:139:MET:HG2	3:P:255:GLU:HB3	1.84	0.60
1:A:161:THR:HG21	1:A:235:ARG:H	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:38:LEU:HB2	10:W:14:PHE:HE1	1.65	0.60
7:T:40:ARG:HD2	15:T:3004:CDL:OA4	2.01	0.60
5:R:52:LYS:HD3	5:R:52:LYS:C	2.22	0.60
3:C:139:MET:HE3	3:C:270:LYS:H	1.67	0.60
4:Q:221:TYR:HD2	5:R:39:VAL:HG11	1.66	0.60
5:R:49:TYR:CE1	10:W:32:GLU:HG3	2.37	0.60
1:A:280:TYR:CG	1:A:281:ASP:N	2.70	0.60
3:P:155:PRO:O	3:P:156:TYR:HB2	2.02	0.60
1:A:206:LYS:O	1:A:209:VAL:HG12	2.00	0.60
1:A:170:THR:CG2	1:A:171:THR:N	2.65	0.59
3:P:278:ALA:HB1	3:P:295:LEU:CD1	2.32	0.59
3:C:36:SER:O	3:C:40:VAL:HG23	2.02	0.59
1:N:231:LEU:CD2	1:N:232:PRO:HD2	2.30	0.59
2:O:47:ILE:HG12	2:O:120:MET:HE3	1.84	0.59
2:B:168:TYR:HB2	2:B:173:ALA:HB2	1.83	0.59
1:N:137:GLU:O	1:N:141:MET:HG3	2.01	0.59
1:N:134:ILE:HG21	1:N:174:ILE:HD13	1.84	0.59
4:Q:76:GLU:CD	4:Q:76:GLU:N	2.56	0.59
6:S:32:MET:CE	6:S:87:LYS:H	2.15	0.59
8:H:21:ARG:O	8:H:25:GLU:HG3	2.02	0.59
1:N:187:ASP:O	1:N:191:LYS:HE3	2.02	0.59
1:N:196:VAL:CG1	1:N:383:LEU:HD12	2.31	0.59
2:O:122:TYR:O	2:O:126:VAL:HG23	2.03	0.59
1:A:13:GLU:HG2	1:A:14:THR:N	2.17	0.59
3:P:143:GLY:HA2	14:P:3001:3H1:H08A	1.85	0.59
3:P:189:ALA:O	3:P:193:ILE:HG13	2.03	0.59
4:Q:240:PRO:HD3	7:T:12:HIS:CE1	2.37	0.59
2:B:31:ASN:N	2:B:31:ASN:HD22	2.01	0.59
1:A:106:MET:HG3	1:A:203:ILE:CG2	2.33	0.59
4:Q:234:LYS:HZ1	5:R:13:TYR:HE2	1.51	0.59
2:B:314:VAL:HG13	9:I:63:ASP:HB3	1.83	0.59
6:S:13:MET:HA	6:S:16:ILE:HB	1.85	0.59
2:O:407:SER:O	2:O:411:VAL:HG23	2.02	0.59
5:R:99:ARG:HB3	5:R:133:VAL:CG1	2.32	0.59
2:O:226:ILE:CG2	2:O:227:ARG:N	2.66	0.59
9:V:55:MET:HA	9:V:58:ARG:HG3	1.84	0.59
3:P:247:SER:OG	3:P:250:LEU:HB2	2.02	0.59
1:A:43:ALA:HB2	1:A:194:ARG:HH21	1.68	0.59
8:U:32:LYS:O	8:U:36:ARG:HG3	2.03	0.59
1:N:49:ASN:ND2	1:N:51:LYS:N	2.51	0.59
3:P:319:ARG:O	3:P:323:GLN:HG3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:SER:OG	1:A:92:ARG:HA	2.03	0.59
7:T:29:ILE:HD12	7:T:29:ILE:N	2.17	0.58
1:A:134:ILE:CG2	1:A:174:ILE:HD13	2.32	0.58
2:B:86:THR:O	2:B:90:GLU:HG3	2.03	0.58
9:I:28:UNK:N	9:I:72:ALA:HB2	2.18	0.58
1:N:39:VAL:HG11	1:N:117:VAL:HG11	1.85	0.58
3:C:132:TYR:OH	3:C:139:MET:HG3	2.03	0.58
3:C:121:LEU:HG	3:C:125:MET:CE	2.33	0.58
2:B:312:PHE:HE1	9:I:62:ARG:O	1.85	0.58
8:H:40:CYS:HA	8:H:43:ARG:NH1	2.17	0.58
7:T:74:PRO:O	7:T:78:GLU:HG3	2.04	0.58
1:A:44:GLY:H	1:A:47:TYR:HD1	1.52	0.58
10:W:30:LEU:HD23	10:W:33:ARG:HH22	1.68	0.58
1:A:95:THR:HG22	1:A:96:ALA:N	2.18	0.58
3:C:332:ASN:HD21	3:C:358:SER:CB	2.16	0.58
6:F:77:LYS:HA	6:F:80:TRP:CE2	2.38	0.58
2:O:181:TYR:CE1	2:O:182:ARG:HG3	2.38	0.58
1:N:40:TRP:CD1	1:N:96:ALA:HB2	2.39	0.58
3:P:23:PRO:HG2	7:T:3:HIS:HB2	1.85	0.58
10:J:49:GLY:N	10:J:54:HIS:ND1	2.52	0.58
2:B:247:GLN:HE22	2:B:429:ASP:HA	1.67	0.58
7:G:36:ASN:OD1	7:G:39:ARG:NH1	2.36	0.58
5:R:77:LYS:HE2	5:R:79:SER:HB2	1.86	0.58
4:Q:29:GLY:HA3	4:Q:189:PHE:HB2	1.85	0.58
3:P:335:ILE:HD13	7:T:58:LEU:HD23	1.84	0.58
6:F:32:MET:HE1	6:F:87:LYS:H	1.68	0.58
3:P:15:ILE:CD1	3:P:15:ILE:H	2.17	0.58
1:A:37:VAL:HG12	1:A:199:ALA:CB	2.33	0.58
3:C:285:ILE:CD1	3:C:285:ILE:H	2.17	0.58
2:B:274:VAL:O	2:B:278:VAL:HG23	2.03	0.58
2:B:229:GLY:O	2:B:231:GLY:N	2.37	0.58
3:C:207:ASN:ND2	3:C:314:ARG:NH1	2.52	0.58
3:C:137:GLY:H	3:C:140:SER:HB2	1.68	0.58
2:B:206:LEU:HD23	2:B:220:ALA:HB2	1.85	0.58
4:Q:116:ILE:HG21	4:Q:190:LEU:HD13	1.86	0.58
2:O:297:GLN:O	2:O:301:LYS:HG3	2.04	0.58
3:C:243:LEU:HD11	3:C:250:LEU:HD23	1.86	0.58
3:C:271:PRO:HD2	3:C:276:LEU:HD23	1.86	0.57
2:O:291:VAL:HA	2:O:297:GLN:NE2	2.19	0.57
2:O:150:VAL:HG23	2:O:151:ALA:N	2.19	0.57
2:B:327:ILE:HD11	9:I:58:ARG:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:LEU:HD12	1:A:392:LEU:HD11	1.86	0.57
3:P:137:GLY:H	3:P:140:SER:HB2	1.70	0.57
7:G:29:ILE:HD12	7:G:29:ILE:N	2.20	0.57
3:C:90:PHE:CE1	3:C:240:PHE:HA	2.40	0.57
2:B:292:THR:O	2:B:292:THR:HG22	2.04	0.57
8:H:16:PRO:O	8:H:20:ILE:HG13	2.04	0.57
1:N:106:MET:HG3	1:N:203:ILE:HG23	1.86	0.57
5:R:69:LEU:HD13	5:R:71:LEU:HD11	1.85	0.57
2:B:202:ALA:HB2	2:B:228:SER:HB2	1.87	0.57
3:P:285:ILE:H	3:P:285:ILE:CD1	2.18	0.57
3:P:285:ILE:H	3:P:285:ILE:HD12	1.69	0.57
4:D:28:ARG:HD2	4:D:171:TYR:CE1	2.39	0.57
1:A:342:TRP:O	1:A:345:LEU:HB2	2.05	0.57
2:O:27:THR:CG2	2:O:28:LYS:N	2.68	0.57
1:A:130:GLU:O	1:A:134:ILE:HG13	2.05	0.57
7:G:74:PRO:O	7:G:78:GLU:HG3	2.04	0.57
9:I:28:UNK:H2	9:I:72:ALA:HB2	1.70	0.57
5:R:122:HIS:CE1	5:R:124:LEU:HG	2.40	0.57
1:A:39:VAL:HG11	1:A:117:VAL:HG11	1.87	0.57
3:C:17:ASN:ND2	7:G:1:GLY:HA2	2.20	0.57
2:O:292:THR:CG2	2:O:363:GLN:HE22	2.15	0.57
3:C:319:ARG:O	3:C:323:GLN:HG3	2.04	0.57
2:O:162:ASN:O	2:O:244:ILE:HD12	2.05	0.57
2:B:169:LYS:O	2:B:170:THR:HG23	2.04	0.57
5:R:161:HIS:HB2	19:R:501:FES:S1	2.44	0.57
3:C:285:ILE:N	3:C:285:ILE:CD1	2.68	0.57
5:R:99:ARG:HB3	5:R:133:VAL:HG13	1.87	0.57
5:E:83:GLU:HG2	5:E:102:THR:HG22	1.86	0.57
4:Q:26:VAL:HG12	4:Q:55:THR:HG21	1.87	0.57
2:O:292:THR:HG22	2:O:292:THR:O	2.05	0.57
2:O:59:THR:HG22	2:O:60:THR:H	1.68	0.57
3:P:332:ASN:HD21	3:P:358:SER:HB3	1.70	0.57
2:B:220:ALA:O	2:B:224:LEU:HB2	2.05	0.56
2:O:327:ILE:HG22	9:V:55:MET:HE3	1.87	0.56
7:G:41:PHE:HD2	7:G:41:PHE:C	2.08	0.56
6:S:104:ARG:O	6:S:108:ASN:ND2	2.38	0.56
4:Q:149:TYR:CE1	4:Q:156:GLN:HB3	2.40	0.56
3:C:139:MET:HG2	3:C:255:GLU:HB3	1.87	0.56
2:B:62:ASN:HA	2:B:190:GLN:NE2	2.19	0.56
2:O:63:LEU:HB2	2:O:182:ARG:CD	2.36	0.56
2:B:27:THR:HG22	2:B:28:LYS:H	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:325:TYR:CD1	9:V:60:ALA:HB2	2.40	0.56
6:F:104:ARG:O	6:F:108:ASN:ND2	2.38	0.56
2:B:277:HIS:NE2	2:B:364:LEU:HD13	2.19	0.56
3:C:132:TYR:CD2	12:C:2010:UNL:O1	2.58	0.56
2:B:157:VAL:O	2:B:157:VAL:HG22	2.06	0.56
1:N:29:GLU:HG3	1:N:203:ILE:O	2.05	0.56
8:U:52:GLU:HG2	8:U:53:GLN:H	1.69	0.56
3:C:332:ASN:HD21	3:C:358:SER:HB3	1.71	0.56
2:B:268:GLU:O	2:B:271:ALA:HB3	2.05	0.56
1:A:170:THR:HG22	1:A:172:GLU:H	1.71	0.56
1:A:196:VAL:CG1	1:A:383:LEU:HD12	2.33	0.56
2:B:133:ARG:HD3	2:B:135:TRP:CZ2	2.41	0.56
1:A:388:ARG:NH2	1:A:388:ARG:HG3	2.20	0.56
17:D:501:HEC:HBA1	17:D:501:HEC:HHA	1.86	0.56
1:N:433:ASP:OD2	1:N:435:ASN:HB2	2.05	0.56
9:I:71:ASN:H	9:I:71:ASN:ND2	1.99	0.56
1:N:61:HIS:CE1	1:N:134:ILE:HG12	2.40	0.56
10:J:55:ILE:HG22	10:J:59:TYR:HE1	1.71	0.56
4:D:203:ARG:NH1	10:J:43:PHE:HD2	2.04	0.56
2:O:102:ARG:HG2	2:O:102:ARG:NH1	2.19	0.56
1:A:395:TRP:HA	1:A:395:TRP:HE3	1.68	0.56
1:A:29:GLU:HG3	1:A:203:ILE:O	2.06	0.56
3:P:95:ILE:HD13	3:P:121:LEU:HD12	1.87	0.56
1:N:138:LEU:HD21	1:N:168:GLU:HB3	1.87	0.56
1:A:178:THR:HG22	1:A:179:ARG:N	2.21	0.56
7:T:41:PHE:C	7:T:41:PHE:HD2	2.09	0.56
5:E:95:PRO:HG3	3:P:263:LEU:CD2	2.36	0.56
2:B:227:ARG:NE	2:B:227:ARG:CA	2.68	0.56
1:A:114:ALA:HB2	1:A:216:PHE:CE2	2.41	0.56
3:C:366:LEU:O	3:C:369:THR:N	2.38	0.56
7:G:73:ASN:HD21	7:G:75:ALA:HB3	1.71	0.56
1:N:388:ARG:NH2	1:N:388:ARG:HG3	2.16	0.55
7:T:46:PHE:O	7:T:50:PRO:HG2	2.06	0.55
5:E:78:LEU:HB3	5:E:132:TRP:CZ2	2.41	0.55
1:A:281:ASP:OD2	1:A:284:PHE:HE1	1.89	0.55
3:P:36:SER:O	3:P:40:VAL:HG23	2.06	0.55
2:B:306:PRO:HA	9:I:52:ARG:CG	2.35	0.55
1:N:134:ILE:CG2	1:N:174:ILE:HD13	2.36	0.55
4:Q:239:PRO:HB2	4:Q:240:PRO:HD2	1.88	0.55
4:Q:134:TYR:CG	4:Q:162:PRO:HG3	2.42	0.55
2:O:172:LEU:HD13	2:O:316:TYR:CD1	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:70:LEU:HD12	6:S:70:LEU:C	2.26	0.55
1:N:49:ASN:HD21	1:N:52:ASN:N	2.04	0.55
4:D:197:GLU:HG2	4:D:198:HIS:H	1.72	0.55
2:B:122:TYR:O	2:B:126:VAL:HG23	2.06	0.55
10:W:55:ILE:HG22	10:W:59:TYR:HE1	1.72	0.55
1:A:133:VAL:O	1:A:137:GLU:HG3	2.06	0.55
3:P:345:GLU:O	3:P:348:PHE:HB2	2.07	0.55
2:O:192:HIS:O	2:O:196:GLN:HG3	2.06	0.55
5:E:164:HIS:CD2	5:E:173:LYS:HD3	2.40	0.55
2:B:31:ASN:N	2:B:31:ASN:ND2	2.55	0.55
2:B:292:THR:CG2	2:B:363:GLN:HE22	2.17	0.55
5:E:95:PRO:HG3	3:P:263:LEU:HD23	1.89	0.55
8:U:12:GLU:HG2	8:U:12:GLU:O	2.07	0.55
3:C:129:PHE:CZ	3:C:147:ILE:HD12	2.41	0.55
1:N:62:LEU:CD2	1:N:130:GLU:HG3	2.36	0.55
5:R:171:ILE:HG22	5:R:179:ASN:OD1	2.06	0.55
2:B:59:THR:HG22	2:B:60:THR:H	1.72	0.55
7:G:29:ILE:HD12	7:G:29:ILE:H	1.70	0.55
3:C:156:TYR:C	3:C:158:GLY:H	2.10	0.55
1:A:138:LEU:HD21	1:A:168:GLU:HB3	1.88	0.55
2:B:189:GLU:O	2:B:192:HIS:N	2.39	0.55
3:P:95:ILE:HD13	3:P:121:LEU:CD1	2.36	0.55
2:O:52:LYS:HB2	2:O:203:ARG:HB3	1.89	0.55
3:C:11:LEU:O	3:C:14:MET:HB2	2.06	0.55
3:C:329:LEU:O	3:C:332:ASN:HB3	2.06	0.55
1:A:406:MET:O	1:A:410:VAL:HG23	2.07	0.55
2:B:34:ILE:HD13	2:B:386:ALA:O	2.07	0.55
2:B:154:SER:O	2:B:157:VAL:HG12	2.06	0.54
4:Q:139:ALA:CB	8:U:41:ASP:HA	2.38	0.54
7:G:29:ILE:CD1	7:G:29:ILE:H	2.20	0.54
7:T:41:PHE:C	7:T:41:PHE:CD2	2.81	0.54
4:D:8:PRO:HG2	4:D:10:PHE:CE1	2.42	0.54
3:C:137:GLY:N	3:C:140:SER:HB2	2.23	0.54
5:E:161:HIS:HB2	19:E:501:FES:S1	2.48	0.54
1:A:106:MET:HG3	1:A:203:ILE:HG23	1.89	0.54
3:P:275:PHE:HB3	14:P:3001:3H1:H16A	1.89	0.54
1:N:236:PHE:HB2	1:N:258:GLU:OE1	2.07	0.54
8:U:21:ARG:O	8:U:25:GLU:HG3	2.08	0.54
3:P:243:LEU:HD11	3:P:250:LEU:HD23	1.90	0.54
7:G:41:PHE:CD2	7:G:41:PHE:C	2.79	0.54
2:O:247:GLN:HE22	2:O:429:ASP:HA	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:144:LEU:HB2	2:B:183:ILE:HD12	1.88	0.54
10:W:14:PHE:CD2	10:W:14:PHE:N	2.73	0.54
3:P:72:ARG:NE	4:Q:115:TYR:OH	2.40	0.54
2:O:344:LEU:HD23	2:O:417:PHE:CE2	2.43	0.54
1:N:133:VAL:O	1:N:137:GLU:HG3	2.08	0.54
10:W:40:ASP:O	10:W:44:GLU:HG3	2.06	0.54
4:D:102:ARG:HB3	4:D:107:GLY:HA2	1.89	0.54
2:B:344:LEU:HD23	2:B:417:PHE:CE2	2.43	0.54
1:N:136:GLN:HE22	9:V:50:LEU:CD1	2.21	0.54
3:P:329:LEU:O	3:P:332:ASN:HB3	2.08	0.54
5:E:77:LYS:HE2	5:E:79:SER:HB2	1.88	0.54
1:N:112:LEU:O	1:N:116:VAL:HG23	2.07	0.54
2:O:229:GLY:O	2:O:231:GLY:N	2.40	0.54
1:N:60:GLU:OE2	1:N:89:TYR:HA	2.07	0.54
2:B:291:VAL:HA	2:B:297:GLN:HE21	1.73	0.54
1:N:281:ASP:OD2	1:N:284:PHE:HE1	1.90	0.54
5:E:101:ARG:HH22	5:E:127:VAL:HG21	1.73	0.54
2:B:157:VAL:CG2	9:I:64:LEU:HD21	2.31	0.54
3:P:285:ILE:N	3:P:285:ILE:CD1	2.71	0.54
2:O:307:PHE:CD1	2:O:308:ASP:N	2.76	0.54
2:B:262:ALA:HB3	2:B:269:ALA:HB2	1.90	0.54
1:A:69:LYS:HE3	1:A:70:ARG:HH21	1.73	0.54
5:R:164:HIS:CD2	5:R:173:LYS:HD3	2.43	0.54
2:B:63:LEU:HB2	2:B:182:ARG:CD	2.38	0.53
1:A:49:ASN:HD21	1:A:52:ASN:N	2.06	0.53
2:B:344:LEU:HD23	2:B:417:PHE:CD2	2.44	0.53
2:O:47:ILE:HG12	2:O:120:MET:CE	2.38	0.53
3:P:219:ILE:HB	3:P:224:TYR:HD1	1.73	0.53
5:E:69:LEU:HD13	5:E:71:LEU:HD11	1.90	0.53
3:C:95:ILE:O	3:C:99:ILE:HG13	2.09	0.53
10:W:58:LYS:HB2	10:W:59:TYR:CE1	2.43	0.53
6:F:31:LEU:HD21	6:F:65:ALA:CB	2.38	0.53
4:Q:215:LEU:HD13	5:R:46:ALA:HB3	1.88	0.53
2:B:29:LEU:CB	2:B:30:PRO:HD2	2.38	0.53
5:E:102:THR:O	5:E:106:ILE:HG13	2.09	0.53
6:S:17:ARG:HG3	6:S:17:ARG:HH11	1.73	0.53
2:O:217:LYS:O	2:O:221:GLU:HG2	2.08	0.53
1:A:131:ARG:NH1	1:A:131:ARG:HG3	2.21	0.53
3:P:145:THR:O	3:P:149:ASN:HB2	2.08	0.53
1:A:62:LEU:HD21	1:A:130:GLU:HG3	1.91	0.53
2:B:172:LEU:HD13	2:B:316:TYR:CD1	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:178:THR:CG2	1:N:179:ARG:N	2.71	0.53
1:N:45:SER:HA	1:N:48:GLU:CD	2.29	0.53
3:C:121:LEU:HG	3:C:125:MET:HE3	1.91	0.53
5:R:77:LYS:HE2	5:R:79:SER:CB	2.38	0.53
3:C:145:THR:O	3:C:149:ASN:HB2	2.09	0.53
5:R:101:ARG:HH22	5:R:127:VAL:HG21	1.74	0.53
5:R:83:GLU:HG2	5:R:102:THR:HG22	1.89	0.53
3:C:19:LEU:O	3:C:20:ILE:CG1	2.53	0.53
3:P:219:ILE:HB	3:P:224:TYR:CD1	2.44	0.53
3:P:137:GLY:N	3:P:140:SER:HB2	2.24	0.53
5:E:95:PRO:HG2	5:E:145:VAL:HG21	1.90	0.53
3:C:377:MET:HE2	6:F:20:TYR:HB2	1.90	0.53
2:B:361:LYS:O	2:B:365:LYS:HG3	2.08	0.53
4:D:150:ASN:O	4:D:156:GLN:HA	2.08	0.53
1:A:209:VAL:O	1:A:213:ARG:HG3	2.09	0.53
6:S:31:LEU:HD21	6:S:65:ALA:CB	2.39	0.53
1:A:233:ARG:HG2	1:A:233:ARG:NH1	2.24	0.53
1:N:178:THR:HG22	1:N:180:ALA:H	1.74	0.53
1:N:62:LEU:HD21	1:N:130:GLU:HG3	1.90	0.53
6:S:32:MET:HE3	6:S:87:LYS:H	1.74	0.53
1:N:111:GLU:HG3	1:N:215:HIS:CD2	2.44	0.53
3:C:5:ILE:HG22	3:C:5:ILE:O	2.09	0.53
8:U:36:ARG:HB2	8:U:36:ARG:HH11	1.73	0.52
1:N:145:MET:HB3	1:N:252:HIS:CD2	2.44	0.52
3:C:180:PHE:HE1	3:P:180:PHE:HE1	1.56	0.52
3:C:157:ILE:O	3:C:161:LEU:HD12	2.09	0.52
2:O:168:TYR:HB2	2:O:173:ALA:HB2	1.90	0.52
7:G:49:ALA:HB3	7:G:50:PRO:HD3	1.92	0.52
1:A:60:GLU:OE2	1:A:89:TYR:HA	2.09	0.52
9:V:32:UNK:C	9:V:73:PRO:HG2	2.39	0.52
3:P:206:SER:OG	14:P:3002:3H1:H08B	2.09	0.52
2:B:181:TYR:CE1	2:B:182:ARG:HG3	2.44	0.52
7:T:48:VAL:HG12	7:T:49:ALA:N	2.22	0.52
1:A:45:SER:HA	1:A:48:GLU:CD	2.30	0.52
1:N:242:ARG:HH22	1:N:432:LEU:HA	1.74	0.52
2:B:354:GLU:O	2:B:358:THR:HG23	2.09	0.52
3:C:285:ILE:H	3:C:285:ILE:HD12	1.72	0.52
1:N:85:HIS:NE2	2:O:284:LEU:HD22	2.24	0.52
2:O:128:THR:HG21	2:O:224:LEU:CD2	2.40	0.52
1:A:49:ASN:ND2	1:A:51:LYS:N	2.58	0.52
3:P:129:PHE:CZ	3:P:147:ILE:HD12	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:29:ILE:O	7:T:33:ALA:HB3	2.08	0.52
7:G:50:PRO:HB2	7:G:51:PRO:HD3	1.91	0.52
1:A:62:LEU:CD2	1:A:130:GLU:HG3	2.40	0.52
3:P:90:PHE:CZ	3:P:240:PHE:HA	2.45	0.52
2:B:168:TYR:CE2	2:B:172:LEU:HD12	2.44	0.52
4:Q:150:ASN:O	4:Q:156:GLN:HA	2.10	0.52
2:B:307:PHE:CD1	2:B:308:ASP:N	2.78	0.52
2:B:68:LEU:HD23	2:B:186:ILE:HG21	1.92	0.52
1:A:106:MET:HE2	1:A:107:PRO:HA	1.92	0.52
5:R:156:TYR:HB2	5:R:165:TYR:HB2	1.90	0.52
7:G:40:ARG:HD2	15:G:2004:CDL:OA4	2.09	0.52
4:D:134:TYR:CG	4:D:162:PRO:HG3	2.45	0.52
2:O:31:ASN:N	2:O:31:ASN:HD22	2.07	0.52
3:C:90:PHE:HB3	3:C:236:MET:CE	2.35	0.52
9:I:59:SER:O	9:I:60:ALA:C	2.48	0.52
2:B:35:ILE:HD13	2:B:217:LYS:HA	1.91	0.52
10:W:59:TYR:N	10:W:59:TYR:CD1	2.77	0.52
5:E:101:ARG:NH2	5:E:127:VAL:HG21	2.25	0.52
1:A:422:LEU:HD22	1:A:437:ILE:HD13	1.92	0.52
1:N:336:PHE:CE2	3:P:4:ASN:HB3	2.45	0.52
3:C:105:TYR:HA	3:C:315:THR:HG22	1.92	0.52
1:A:49:ASN:ND2	1:A:51:LYS:H	2.08	0.52
2:O:268:GLU:O	2:O:268:GLU:HG2	2.10	0.52
2:B:202:ALA:HB2	2:B:229:GLY:H	1.75	0.52
8:H:17:LEU:HD13	8:H:73:LEU:CD2	2.40	0.52
3:C:332:ASN:ND2	3:C:358:SER:OG	2.43	0.52
7:T:41:PHE:HD2	7:T:41:PHE:O	1.92	0.52
3:P:5:ILE:O	3:P:5:ILE:HG22	2.10	0.52
2:O:22:GLU:HG3	2:O:39:GLU:CB	2.37	0.52
2:O:62:ASN:HA	2:O:190:GLN:NE2	2.25	0.52
5:E:141:HIS:O	5:E:142:LEU:HD23	2.10	0.52
7:T:65:GLU:O	7:T:69:LEU:HG	2.10	0.52
2:B:303:THR:HA	2:B:335:GLU:OE2	2.11	0.51
6:S:76:PRO:O	6:S:78:GLU:N	2.44	0.51
3:C:187:PRO:O	3:C:190:ILE:HB	2.10	0.51
2:B:248:ASN:ND2	2:B:248:ASN:C	2.63	0.51
1:A:117:VAL:HG23	1:A:118:GLN:HG3	1.91	0.51
3:C:377:MET:HE1	6:F:20:TYR:CD1	2.45	0.51
2:B:150:VAL:HG23	2:B:151:ALA:N	2.25	0.51
2:B:259:THR:HG22	2:B:260:GLU:N	2.24	0.51
4:D:223:LYS:HD3	4:D:223:LYS:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:47:ILE:N	2:B:47:ILE:CD1	2.73	0.51
1:N:321:GLY:HA2	1:N:342:TRP:HZ2	1.75	0.51
3:C:247:SER:OG	3:C:250:LEU:HB2	2.10	0.51
2:B:327:ILE:HG22	9:I:55:MET:HE3	1.91	0.51
1:N:156:THR:HA	5:R:7:VAL:HG21	1.92	0.51
1:A:305:HIS:ND1	9:I:35:UNK:CB	2.74	0.51
3:P:81:ARG:HH11	3:P:81:ARG:HG3	1.75	0.51
8:U:52:GLU:CG	8:U:53:GLN:N	2.74	0.51
3:P:271:PRO:HD2	3:P:276:LEU:HD23	1.91	0.51
1:N:433:ASP:OD2	1:N:435:ASN:N	2.43	0.51
2:B:262:ALA:CB	2:B:269:ALA:HB2	2.39	0.51
5:R:101:ARG:NH2	5:R:127:VAL:HG21	2.26	0.51
5:R:102:THR:O	5:R:106:ILE:HG13	2.09	0.51
2:B:403:ASP:C	2:B:405:VAL:H	2.13	0.51
1:A:187:ASP:O	1:A:191:LYS:HE3	2.10	0.51
3:P:212:ILE:HD12	6:S:62:ILE:HG23	1.92	0.51
4:D:14:HIS:CG	4:D:21:LEU:HD23	2.45	0.51
4:D:37:CYS:C	4:D:39:ALA:H	2.12	0.51
2:B:102:ARG:HG2	2:B:102:ARG:NH1	2.23	0.51
1:N:45:SER:HA	1:N:48:GLU:CG	2.41	0.51
1:N:246:ASP:HA	1:N:427:PRO:HB3	1.91	0.51
7:T:36:ASN:OD1	7:T:39:ARG:NH1	2.42	0.51
3:C:167:GLY:HA3	3:C:178:ARG:NH2	2.25	0.51
3:P:11:LEU:O	3:P:14:MET:HB2	2.10	0.51
2:O:259:THR:CG2	2:O:260:GLU:N	2.73	0.51
8:U:72:LYS:HA	8:U:75:ASN:ND2	2.24	0.51
1:A:10:ASN:HD21	2:B:19:PRO:HD3	1.75	0.51
6:S:40:ASP:O	6:S:44:LYS:HG3	2.11	0.51
3:P:32:TRP:NE1	13:P:502:HEM:O2D	2.42	0.51
3:C:70:THR:O	3:C:74:VAL:HB	2.10	0.51
2:O:403:ASP:C	2:O:405:VAL:H	2.14	0.51
8:U:51:GLU:O	8:U:51:GLU:HG3	2.10	0.51
10:J:40:ASP:O	10:J:44:GLU:HG3	2.11	0.51
2:O:376:GLN:HE22	9:V:77:ARG:NH2	2.06	0.51
1:N:136:GLN:HG2	9:V:51:CYS:HB3	1.92	0.51
4:Q:229:VAL:CG2	7:T:20:PRO:HG3	2.39	0.51
5:R:78:LEU:HB3	5:R:132:TRP:CZ2	2.46	0.51
1:N:95:THR:HG22	1:N:96:ALA:N	2.25	0.51
1:N:45:SER:OG	1:N:92:ARG:HA	2.11	0.51
8:U:36:ARG:NH1	8:U:36:ARG:HB2	2.26	0.51
4:D:131:LEU:HD11	17:D:501:HEC:HMB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:50:PRO:HB2	7:T:51:PRO:HD3	1.93	0.51
1:A:93:GLU:O	1:A:94:GLN:HB2	2.09	0.51
4:Q:181:GLN:HA	8:U:77:LEU:HD22	1.92	0.51
1:N:422:LEU:HD22	1:N:437:ILE:HD13	1.93	0.51
1:A:276:ILE:HG12	1:A:357:ALA:HB2	1.93	0.51
3:C:278:ALA:HB1	3:C:295:LEU:CD1	2.41	0.51
3:C:289:LEU:HD12	3:C:289:LEU:O	2.11	0.51
4:Q:14:HIS:CG	4:Q:21:LEU:HD23	2.46	0.51
4:Q:223:LYS:O	4:Q:223:LYS:HD3	2.10	0.51
3:P:92:PHE:HA	3:P:95:ILE:HG22	1.93	0.51
1:N:117:VAL:HG23	1:N:118:GLN:HG3	1.94	0.51
7:G:41:PHE:O	7:G:41:PHE:HD2	1.94	0.51
4:Q:203:ARG:HD2	18:R:3009:BOG:O6	2.11	0.51
3:C:105:TYR:CA	3:C:315:THR:HG22	2.41	0.51
2:B:407:SER:O	2:B:411:VAL:HG23	2.10	0.51
3:P:31:TRP:O	3:P:101:ARG:HG3	2.11	0.50
7:T:73:ASN:ND2	7:T:75:ALA:HB3	2.26	0.50
4:D:240:PRO:HD3	7:G:12:HIS:NE2	2.26	0.50
3:C:172:ASP:OD1	3:C:173:ASN:N	2.35	0.50
3:C:272:GLU:HA	3:C:272:GLU:OE1	2.10	0.50
3:P:242:THR:N	4:Q:208:MET:HE1	2.25	0.50
7:G:81:GLN:OXT	8:H:49:HIS:HB3	2.11	0.50
3:P:139:MET:CE	3:P:270:LYS:H	2.23	0.50
6:F:91:GLU:O	6:F:95:LYS:HG3	2.11	0.50
3:P:105:TYR:CD2	3:P:209:PRO:HA	2.46	0.50
1:A:67:THR:HG21	1:A:115:ASP:OD2	2.10	0.50
3:P:183:HIS:O	3:P:187:PRO:HD2	2.12	0.50
3:C:106:GLY:HA2	3:C:108:TYR:CE2	2.45	0.50
3:P:36:SER:HA	14:P:3002:3H1:H16B	1.92	0.50
1:N:13:GLU:HG2	1:N:14:THR:N	2.26	0.50
1:N:69:LYS:HE3	1:N:70:ARG:HH21	1.77	0.50
4:Q:2:GLU:HG2	4:Q:2:GLU:O	2.11	0.50
8:U:13:LEU:H	8:U:13:LEU:HD23	1.77	0.50
7:G:48:VAL:HG12	7:G:49:ALA:N	2.24	0.50
1:A:95:THR:HG22	1:A:96:ALA:H	1.76	0.50
2:B:262:ALA:O	2:B:320:GLY:HA3	2.11	0.50
1:A:369:LEU:CD1	1:A:392:LEU:HD21	2.41	0.50
5:E:77:LYS:HE2	5:E:79:SER:CB	2.41	0.50
4:D:221:TYR:CD2	5:E:39:VAL:HG11	2.47	0.50
2:O:303:THR:HA	2:O:335:GLU:OE2	2.10	0.50
5:R:141:HIS:O	5:R:142:LEU:HD23	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:67:HIS:O	2:B:70:ARG:HB3	2.12	0.50
3:P:13:LYS:HG2	3:P:13:LYS:O	2.11	0.50
1:N:40:TRP:HZ3	1:N:376:CYS:HG	1.56	0.50
2:O:47:ILE:CD1	2:O:47:ILE:N	2.74	0.50
1:N:79:VAL:O	1:N:82:MET:HG2	2.11	0.50
10:J:30:LEU:HD23	10:J:33:ARG:HH22	1.77	0.50
1:A:241:ILE:HG23	1:A:241:ILE:O	2.10	0.50
2:B:207:VAL:HG21	2:B:383:GLY:HA2	1.93	0.50
4:Q:57:THR:CG2	10:W:59:TYR:HB2	2.42	0.50
5:E:38:LEU:HB2	10:J:14:PHE:HE1	1.76	0.50
3:P:139:MET:HE3	3:P:270:LYS:O	2.12	0.49
2:O:62:ASN:O	2:O:65:THR:CG2	2.57	0.49
1:N:93:GLU:O	1:N:94:GLN:HB2	2.12	0.49
2:O:422:LYS:O	2:O:436:LEU:HD21	2.12	0.49
3:P:9:HIS:O	3:P:13:LYS:HB3	2.12	0.49
8:U:16:PRO:O	8:U:20:ILE:HG13	2.12	0.49
3:C:236:MET:HB2	15:C:2003:CDL:H161	1.94	0.49
5:E:122:HIS:CE1	5:E:124:LEU:HG	2.46	0.49
3:C:34:PHE:HB2	20:C:381:HOH:O	2.12	0.49
2:O:295:LEU:HA	2:O:343:GLN:HG2	1.95	0.49
1:A:45:SER:HA	1:A:48:GLU:HG3	1.93	0.49
2:O:42:SER:OG	2:O:43:PRO:HD2	2.13	0.49
6:S:10:GLY:C	6:S:12:LEU:H	2.15	0.49
1:A:433:ASP:OD2	1:A:435:ASN:HB2	2.13	0.49
6:F:53:ASP:OD1	6:F:54:LEU:N	2.45	0.49
2:O:128:THR:HG21	2:O:224:LEU:HD22	1.94	0.49
3:P:139:MET:HE3	3:P:270:LYS:H	1.76	0.49
2:B:33:LEU:CD2	2:B:224:LEU:HD12	2.40	0.49
1:A:112:LEU:O	1:A:116:VAL:HG23	2.12	0.49
10:J:14:PHE:CD2	10:J:14:PHE:N	2.76	0.49
2:B:275:LEU:O	2:B:279:LEU:HD12	2.13	0.49
6:S:61:ARG:NH2	6:S:89:TYR:CE2	2.81	0.49
10:J:17:THR:O	10:J:17:THR:HG22	2.12	0.49
2:B:24:LEU:HD21	2:B:392:HIS:CD2	2.48	0.49
4:Q:203:ARG:HD3	10:W:40:ASP:OD1	2.13	0.49
6:F:42:ASP:OD2	6:F:101:ARG:NH1	2.45	0.49
3:C:13:LYS:HG2	3:C:13:LYS:O	2.11	0.49
2:B:76:THR:HG22	2:B:81:SER:HA	1.92	0.49
2:O:221:GLU:HG3	2:O:222:GLN:N	2.20	0.49
2:O:248:ASN:C	2:O:248:ASN:ND2	2.63	0.49
1:A:40:TRP:HZ3	1:A:376:CYS:HG	1.58	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:87:ASN:ND2	1:N:98:TYR:OH	2.45	0.49
4:Q:70:VAL:HG21	4:Q:85:GLY:HA2	1.94	0.49
1:A:295:ALA:O	1:A:299:VAL:HG23	2.12	0.49
3:P:121:LEU:HG	3:P:125:MET:CE	2.42	0.49
2:O:275:LEU:O	2:O:279:LEU:HD12	2.12	0.49
2:O:154:SER:O	2:O:157:VAL:HG12	2.13	0.49
2:B:33:LEU:HD12	2:B:204:MET:O	2.12	0.49
2:B:306:PRO:HB3	9:I:52:ARG:N	2.27	0.49
3:P:112:GLU:O	3:P:116:THR:HG23	2.13	0.49
6:F:71:LYS:O	6:F:72:HIS:HB2	2.12	0.49
2:O:42:SER:O	2:O:113:ARG:HD2	2.13	0.49
4:Q:182:ILE:HG22	4:Q:183:ALA:N	2.28	0.49
9:V:67:GLY:O	9:V:68:ILE:HD13	2.13	0.49
8:H:58:LEU:HD11	8:H:62:LEU:HD11	1.95	0.49
4:D:218:LEU:HD13	5:E:43:ALA:N	2.28	0.49
7:T:49:ALA:HB3	7:T:50:PRO:HD3	1.95	0.49
7:T:41:PHE:CE2	7:T:45:VAL:HB	2.48	0.49
1:N:336:PHE:CZ	3:P:4:ASN:HB3	2.48	0.49
1:A:228:VAL:O	1:A:228:VAL:HG13	2.12	0.49
2:O:76:THR:HG23	2:O:82:SER:HB2	1.94	0.48
2:B:207:VAL:HG12	2:B:208:GLY:N	2.21	0.48
3:P:90:PHE:HB3	3:P:236:MET:HE1	1.94	0.48
3:C:23:PRO:HG2	7:G:3:HIS:HB2	1.94	0.48
11:P:3007:PEE:H7	7:T:44:GLN:HE21	1.78	0.48
1:N:228:VAL:O	1:N:228:VAL:HG13	2.13	0.48
1:A:136:GLN:HE21	9:I:50:LEU:HB2	1.78	0.48
2:O:157:VAL:HG22	2:O:157:VAL:O	2.13	0.48
1:A:321:GLY:HA2	1:A:342:TRP:HZ2	1.78	0.48
1:N:86:PHE:CD1	1:N:99:ILE:HG12	2.48	0.48
4:Q:102:ARG:HB3	4:Q:107:GLY:HA2	1.95	0.48
2:O:354:GLU:O	2:O:358:THR:HG23	2.13	0.48
1:N:106:MET:HE2	1:N:107:PRO:HA	1.95	0.48
5:R:166:ASP:OD1	5:R:168:SER:HB3	2.13	0.48
5:E:77:LYS:HE2	5:E:79:SER:HG	1.78	0.48
5:E:186:GLN:NE2	5:E:188:VAL:CG1	2.76	0.48
3:P:207:ASN:ND2	3:P:208:ASN:H	2.11	0.48
10:W:26:LEU:HD13	10:W:26:LEU:O	2.13	0.48
1:N:295:ALA:O	1:N:298:ALA:HB3	2.12	0.48
2:O:50:PHE:HD2	2:O:104:LYS:NZ	2.08	0.48
2:O:327:ILE:CG2	9:V:55:MET:HE3	2.43	0.48
3:C:137:GLY:H	3:C:140:SER:CB	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:55:MET:O	9:I:58:ARG:HG2	2.14	0.48
2:O:46:ARG:HG2	2:O:379:LEU:HD22	1.95	0.48
3:C:366:LEU:O	3:C:367:PHE:C	2.52	0.48
4:D:116:ILE:CG2	4:D:117:VAL:N	2.76	0.48
1:N:280:TYR:CG	1:N:281:ASP:N	2.81	0.48
5:R:77:LYS:CE	5:R:79:SER:HB2	2.44	0.48
2:B:318:ASP:O	2:B:319:SER:HB2	2.13	0.48
2:O:159:VAL:HG23	2:O:160:LEU:HD23	1.95	0.48
5:R:95:PRO:HG2	5:R:145:VAL:HG21	1.94	0.48
3:P:63:ALA:HB2	3:P:176:LEU:HD21	1.96	0.48
9:I:31:UNK:C	9:I:73:PRO:HG2	2.43	0.48
2:B:62:ASN:O	2:B:65:THR:CG2	2.58	0.48
1:A:178:THR:HG22	1:A:180:ALA:H	1.79	0.48
4:Q:203:ARG:NH1	10:W:43:PHE:HD2	2.12	0.48
3:C:377:MET:HE1	6:F:20:TYR:HD1	1.78	0.48
7:G:65:GLU:O	7:G:69:LEU:HG	2.14	0.48
7:G:2:ILE:HG13	7:G:2:ILE:O	2.13	0.48
1:A:398:ARG:HG2	1:A:398:ARG:NH1	2.27	0.48
5:R:48:ALA:HB1	11:R:3005:PEE:H71	1.96	0.48
2:O:259:THR:O	2:O:260:GLU:C	2.51	0.48
1:A:206:LYS:HA	1:A:209:VAL:HG12	1.94	0.48
3:C:137:GLY:O	3:C:140:SER:HB2	2.14	0.48
7:T:63:THR:HG22	7:T:64:GLN:N	2.29	0.48
2:O:357:VAL:HG12	2:O:361:LYS:HE3	1.95	0.48
1:A:40:TRP:CD1	1:A:96:ALA:HB2	2.49	0.48
2:O:264:VAL:HG23	2:O:316:TYR:C	2.34	0.48
3:P:105:TYR:CE2	3:P:209:PRO:HA	2.49	0.48
6:S:12:LEU:O	6:S:15:ARG:HG2	2.13	0.48
2:B:50:PHE:HD2	2:B:104:LYS:NZ	2.12	0.48
6:F:32:MET:HE3	6:F:87:LYS:N	2.25	0.48
2:B:200:THR:OG1	2:B:203:ARG:HD3	2.14	0.48
2:O:71:LEU:CD1	2:O:144:LEU:HD23	2.44	0.48
2:B:291:VAL:HA	2:B:297:GLN:NE2	2.28	0.48
5:R:49:TYR:HE1	10:W:32:GLU:HG3	1.77	0.48
5:R:119:ASP:HB3	5:R:179:ASN:ND2	2.29	0.48
5:E:144:CYS:HB2	5:E:158:CYS:SG	2.54	0.48
4:Q:138:PRO:HD3	8:U:58:LEU:HD23	1.95	0.48
10:J:38:GLY:O	10:J:42:ILE:HG13	2.14	0.48
1:N:106:MET:HE1	1:N:208:LEU:HA	1.95	0.47
2:B:306:PRO:CG	9:I:51:CYS:HA	2.44	0.47
4:D:57:THR:CG2	10:J:59:TYR:HB2	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:218:LEU:HD11	5:R:42:THR:HG22	1.96	0.47
1:N:439:SER:HA	1:N:442:TYR:CE2	2.48	0.47
4:D:232:SER:HB3	7:G:23:GLN:HE22	1.79	0.47
1:N:270:LEU:HD22	1:N:320:PHE:CE1	2.49	0.47
5:E:171:ILE:HG22	5:E:179:ASN:OD1	2.13	0.47
3:P:18:SER:O	3:P:19:LEU:HG	2.14	0.47
3:C:90:PHE:CZ	3:C:240:PHE:HA	2.49	0.47
8:U:52:GLU:CG	8:U:53:GLN:H	2.28	0.47
3:C:263:LEU:CD2	5:R:95:PRO:HG3	2.43	0.47
3:P:164:TRP:O	3:P:167:GLY:N	2.47	0.47
2:B:26:ILE:O	2:B:26:ILE:HG12	2.12	0.47
4:Q:14:HIS:CB	4:Q:21:LEU:HD23	2.44	0.47
1:N:375:VAL:O	1:N:379:ILE:HD12	2.14	0.47
2:O:291:VAL:C	2:O:293:SER:H	2.16	0.47
4:D:102:ARG:HG2	4:D:102:ARG:HH11	1.78	0.47
4:Q:37:CYS:C	4:Q:39:ALA:H	2.18	0.47
6:S:71:LYS:O	6:S:72:HIS:HB2	2.15	0.47
3:P:52:LEU:HD13	13:P:501:HEM:O2D	2.15	0.47
2:B:27:THR:CG2	2:B:28:LYS:N	2.77	0.47
2:B:280:GLY:HA3	2:B:293:SER:OG	2.14	0.47
4:Q:116:ILE:CG2	4:Q:117:VAL:N	2.78	0.47
1:A:270:LEU:HD22	1:A:320:PHE:CE1	2.49	0.47
2:O:158:GLY:O	2:O:162:ASN:ND2	2.47	0.47
4:Q:24:SER:OG	10:W:55:ILE:HD11	2.15	0.47
1:A:304:CYS:HB2	1:A:325:VAL:O	2.13	0.47
2:O:318:ASP:O	2:O:319:SER:HB2	2.14	0.47
3:C:333:LEU:HD21	3:C:359:TYR:CE1	2.49	0.47
8:H:72:LYS:HA	8:H:75:ASN:ND2	2.29	0.47
2:B:207:VAL:HG21	2:B:383:GLY:CA	2.44	0.47
6:S:31:LEU:HD21	6:S:65:ALA:HB2	1.95	0.47
5:E:119:ASP:HB3	5:E:179:ASN:ND2	2.29	0.47
3:C:219:ILE:HD12	3:C:224:TYR:CD1	2.49	0.47
6:F:70:LEU:HD12	6:F:70:LEU:C	2.35	0.47
3:C:9:HIS:O	3:C:13:LYS:HB3	2.14	0.47
1:N:130:GLU:O	1:N:134:ILE:HG13	2.15	0.47
3:P:271:PRO:HB3	14:P:3001:3H1:CL12	2.52	0.47
8:U:17:LEU:O	8:U:21:ARG:HG3	2.14	0.47
2:B:146:VAL:HG12	2:B:147:ASP:N	2.30	0.47
3:P:187:PRO:O	3:P:190:ILE:HB	2.15	0.47
4:Q:171:TYR:OH	4:Q:182:ILE:HA	2.15	0.47
3:C:219:ILE:HB	3:C:224:TYR:CD1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:41:CYS:HB3	3:P:91:PHE:CD2	2.49	0.47
4:Q:12:TRP:NE1	4:Q:125:ASP:OD2	2.45	0.47
5:E:30:GLU:HB2	10:J:7:ARG:HG2	1.96	0.47
1:A:248:LEU:HB3	1:A:249:PRO:HD2	1.97	0.47
4:Q:95:TYR:CD2	4:Q:101:ALA:HA	2.50	0.47
3:C:189:ALA:O	3:C:193:ILE:HG13	2.15	0.47
3:C:18:SER:O	3:C:19:LEU:HG	2.13	0.47
5:E:103:GLN:O	5:E:107:ASN:ND2	2.48	0.47
1:A:178:THR:CG2	1:A:179:ARG:N	2.78	0.47
2:O:258:VAL:CG2	2:O:321:LEU:HD22	2.45	0.47
3:C:160:THR:O	3:C:163:GLU:N	2.48	0.47
4:D:165:TYR:CE2	4:D:168:ILE:HG13	2.50	0.47
2:B:192:HIS:O	2:B:196:GLN:HG3	2.14	0.47
2:B:312:PHE:CE1	9:I:62:ARG:O	2.68	0.47
1:N:307:PHE:HA	1:N:323:HIS:O	2.15	0.47
4:D:65:ALA:O	4:D:85:GLY:HA3	2.15	0.47
8:H:9:GLU:C	8:H:10:GLU:HG3	2.34	0.47
1:A:7:THR:HG21	2:B:113:ARG:CD	2.45	0.47
3:C:20:ILE:HG22	3:C:21:ASP:OD1	2.15	0.46
1:A:86:PHE:CD1	1:A:99:ILE:HG12	2.49	0.46
5:R:30:GLU:CB	10:W:7:ARG:HG2	2.45	0.46
5:E:83:GLU:HA	5:E:100:HIS:CG	2.49	0.46
2:B:159:VAL:HG23	2:B:160:LEU:HD23	1.97	0.46
2:O:146:VAL:HG12	2:O:147:ASP:N	2.28	0.46
2:O:239:TYR:CD2	2:O:240:TRP:N	2.83	0.46
1:N:294:LEU:HD11	1:N:334:MET:CE	2.45	0.46
3:P:19:LEU:O	3:P:20:ILE:CG1	2.53	0.46
2:B:31:ASN:HB3	2:B:227:ARG:HH22	1.79	0.46
3:P:342:GLN:HE21	3:P:342:GLN:CA	2.21	0.46
1:N:236:PHE:CB	1:N:258:GLU:OE1	2.64	0.46
2:O:258:VAL:HG21	2:O:321:LEU:HD22	1.97	0.46
8:H:18:THR:O	8:H:22:GLU:HG3	2.15	0.46
3:P:226:SER:O	3:P:230:ILE:HG12	2.16	0.46
7:G:63:THR:HG22	7:G:64:GLN:N	2.30	0.46
3:P:138:GLN:HB2	3:P:255:GLU:O	2.16	0.46
3:P:121:LEU:HG	3:P:125:MET:HE3	1.96	0.46
5:E:52:LYS:CD	5:E:52:LYS:C	2.84	0.46
1:N:281:ASP:OD2	1:N:284:PHE:CE1	2.68	0.46
4:Q:234:LYS:HD2	5:R:10:PHE:CE2	2.50	0.46
2:O:325:TYR:CD1	9:V:60:ALA:CB	2.99	0.46
1:A:191:LYS:CA	1:A:195:MET:HE2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:394:ALA:C	2:B:396:SER:H	2.17	0.46
5:E:86:ASN:ND2	5:E:148:ALA:HB2	2.30	0.46
5:R:18:VAL:HG23	5:R:18:VAL:O	2.14	0.46
13:C:501:HEM:HBC2	13:C:501:HEM:HMC2	1.97	0.46
2:O:71:LEU:HD11	2:O:144:LEU:HD23	1.98	0.46
5:R:129:LYS:HG3	5:R:187:PHE:CE2	2.51	0.46
5:R:103:GLN:O	5:R:107:ASN:ND2	2.48	0.46
5:R:144:CYS:HB2	5:R:158:CYS:SG	2.56	0.46
3:P:338:TRP:NE1	7:T:59:TYR:CE1	2.84	0.46
2:O:206:LEU:CD2	2:O:220:ALA:HB2	2.29	0.46
13:C:501:HEM:HBC2	13:C:501:HEM:CMC	2.44	0.46
3:C:345:GLU:O	3:C:348:PHE:HB2	2.14	0.46
2:B:305:GLN:HB3	2:B:306:PRO:HD2	1.98	0.46
3:C:4:ASN:OD1	3:C:7:LYS:HD2	2.16	0.46
5:R:166:ASP:OD2	5:R:170:ARG:HB2	2.16	0.46
5:E:78:LEU:HB3	5:E:132:TRP:CH2	2.51	0.46
2:O:309:ALA:HA	2:O:325:TYR:O	2.16	0.46
5:E:171:ILE:HD13	5:E:176:ALA:HB3	1.98	0.46
3:C:242:THR:N	4:D:208:MET:HE1	2.31	0.46
3:C:275:PHE:HB3	14:C:2001:3H1:H16A	1.97	0.46
3:C:362:ILE:HA	3:C:366:LEU:HB2	1.98	0.46
1:N:204:SER:HB3	1:N:207:GLU:HB2	1.98	0.46
4:D:14:HIS:CB	4:D:21:LEU:HD23	2.46	0.46
4:D:37:CYS:C	4:D:39:ALA:N	2.69	0.46
2:O:67:HIS:O	2:O:70:ARG:HB3	2.15	0.46
2:O:209:ILE:HG13	2:O:379:LEU:HD13	1.97	0.46
2:O:76:THR:HG22	2:O:81:SER:HA	1.97	0.46
2:O:181:TYR:CZ	2:O:182:ARG:HG3	2.51	0.46
3:P:327:TRP:CE2	7:T:48:VAL:HG22	2.50	0.46
2:B:357:VAL:HG12	2:B:361:LYS:HE3	1.97	0.46
2:B:258:VAL:HG21	2:B:321:LEU:HD22	1.96	0.46
1:A:156:THR:HA	5:E:7:VAL:HG21	1.98	0.46
4:Q:169:LEU:HG	4:Q:170:GLU:N	2.30	0.46
2:B:305:GLN:HB3	2:B:306:PRO:CD	2.46	0.46
1:N:131:ARG:HG3	1:N:131:ARG:NH1	2.27	0.46
1:A:106:MET:HE1	1:A:208:LEU:HA	1.97	0.46
5:R:77:LYS:HB3	5:R:80:ASP:OD2	2.16	0.46
4:Q:28:ARG:HD2	4:Q:171:TYR:CE1	2.51	0.46
4:Q:105:ASN:O	4:Q:106:ASN:HB2	2.15	0.46
5:E:126:ARG:O	5:E:182:VAL:HG11	2.16	0.46
2:O:56:ARG:HE	2:O:171:ALA:HB1	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:SER:HB2	1:A:226:ASP:OD1	2.16	0.46
3:P:132:TYR:OH	3:P:139:MET:HG3	2.16	0.46
1:N:382:HIS:CE1	1:N:390:ILE:HB	2.51	0.46
2:B:52:LYS:HB2	2:B:203:ARG:HB3	1.98	0.46
3:P:137:GLY:H	3:P:140:SER:CB	2.28	0.46
1:N:270:LEU:HD13	1:N:320:PHE:CD1	2.51	0.46
3:C:143:GLY:HA2	14:C:2001:3H1:H08A	1.98	0.46
1:A:327:ASP:HB3	1:A:328:PRO:HD2	1.98	0.46
1:A:317:THR:OG1	1:A:318:GLY:N	2.49	0.46
1:N:49:ASN:HD21	1:N:51:LYS:N	2.13	0.45
5:R:193:VAL:HG22	5:R:194:VAL:N	2.31	0.45
5:R:45:VAL:HG13	10:W:28:ALA:CA	2.44	0.45
8:U:36:ARG:NH1	8:U:36:ARG:CB	2.80	0.45
5:R:83:GLU:HA	5:R:100:HIS:CG	2.52	0.45
3:P:81:ARG:NH1	3:P:81:ARG:HG3	2.31	0.45
6:S:12:LEU:C	6:S:14:ASP:H	2.19	0.45
1:N:406:MET:O	1:N:410:VAL:HG23	2.16	0.45
2:O:86:THR:O	2:O:90:GLU:HG3	2.15	0.45
4:D:62:LYS:O	4:D:66:GLU:HG3	2.16	0.45
3:P:270:LYS:HD2	3:P:340:GLY:O	2.16	0.45
2:O:35:ILE:HD13	2:O:217:LYS:HA	1.97	0.45
3:C:342:GLN:HE21	3:C:343:PRO:CD	2.28	0.45
2:B:306:PRO:HG2	9:I:51:CYS:HA	1.98	0.45
7:G:46:PHE:O	7:G:50:PRO:HG2	2.15	0.45
8:H:17:LEU:HD13	8:H:73:LEU:HD22	1.98	0.45
1:A:203:ILE:HG22	1:A:204:SER:N	2.32	0.45
2:B:163:LEU:O	2:B:166:ALA:N	2.49	0.45
10:J:59:TYR:CD1	10:J:59:TYR:N	2.85	0.45
7:G:73:ASN:ND2	7:G:75:ALA:HB3	2.32	0.45
5:E:77:LYS:CE	5:E:79:SER:HB2	2.46	0.45
3:P:105:TYR:CA	3:P:315:THR:HG22	2.46	0.45
2:B:50:PHE:CD1	2:B:50:PHE:N	2.84	0.45
4:Q:138:PRO:HB3	8:U:58:LEU:HD22	1.98	0.45
9:I:71:ASN:N	9:I:71:ASN:ND2	2.51	0.45
2:O:18:CYS:HB3	2:O:19:PRO:HD2	1.99	0.45
2:B:59:THR:CG2	2:B:60:THR:N	2.80	0.45
6:F:61:ARG:HH21	6:F:89:TYR:HE2	1.63	0.45
2:B:258:VAL:CG2	2:B:321:LEU:HD22	2.46	0.45
5:E:186:GLN:HE21	5:E:188:VAL:HG12	1.80	0.45
2:O:348:ALA:HA	2:O:414:ALA:HB3	1.98	0.45
3:C:28:ILE:HG13	3:C:225:TYR:CE2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:38:LEU:O	2:O:38:LEU:HG	2.16	0.45
1:N:182:LEU:HD23	1:N:182:LEU:N	2.32	0.45
3:C:99:ILE:HG12	13:C:502:HEM:HBC2	1.97	0.45
4:Q:165:TYR:CE2	4:Q:168:ILE:HG13	2.51	0.45
3:C:313:GLN:NE2	6:F:36:THR:OG1	2.45	0.45
2:B:241:GLY:HA2	2:B:423:SER:OG	2.16	0.45
4:D:139:ALA:HB3	8:H:54:CYS:SG	2.57	0.45
5:R:186:GLN:HE21	5:R:188:VAL:CG1	2.26	0.45
2:O:249:GLY:O	2:O:250:HIS:C	2.54	0.45
1:N:281:ASP:O	1:N:283:THR:N	2.50	0.45
1:A:43:ALA:HA	1:A:47:TYR:CD1	2.50	0.45
5:E:77:LYS:HB3	5:E:80:ASP:OD2	2.16	0.45
4:D:138:PRO:HB3	8:H:58:LEU:HD22	1.98	0.45
1:N:298:ALA:HA	1:N:303:LEU:HB2	1.98	0.45
2:O:163:LEU:O	2:O:166:ALA:N	2.49	0.45
7:G:53:LEU:O	7:G:57:LEU:HG	2.17	0.45
2:O:156:GLN:HE22	9:V:77:ARG:C	2.20	0.45
8:U:73:LEU:HD12	8:U:73:LEU:C	2.35	0.45
2:O:130:PRO:HB2	2:O:132:PHE:CZ	2.51	0.45
2:B:29:LEU:HB3	2:B:30:PRO:CD	2.44	0.45
2:O:150:VAL:CG2	2:O:151:ALA:N	2.80	0.45
4:D:203:ARG:HD2	18:D:2009:BOG:C6	2.47	0.45
2:O:268:GLU:HG2	2:O:272:PHE:CE1	2.52	0.45
3:P:333:LEU:HD11	11:P:3007:PEE:H38	1.98	0.45
4:Q:165:TYR:O	4:Q:168:ILE:HB	2.17	0.45
1:A:146:THR:HG23	1:A:323:HIS:CE1	2.52	0.45
1:A:307:PHE:C	1:A:307:PHE:CD1	2.89	0.45
2:B:249:GLY:O	2:B:250:HIS:C	2.54	0.45
1:A:3:THR:O	1:A:4:TYR:C	2.55	0.45
1:A:99:ILE:HG13	1:A:113:LEU:HD21	1.98	0.45
1:N:43:ALA:HB2	1:N:194:ARG:HH21	1.81	0.45
2:O:163:LEU:O	2:O:165:ALA:N	2.50	0.45
9:V:39:UNK:O	9:V:40:UNK:C	2.64	0.45
3:P:157:ILE:O	3:P:158:GLY:C	2.54	0.45
2:O:29:LEU:CB	2:O:30:PRO:HD2	2.42	0.45
1:A:64:PHE:HE2	1:A:86:PHE:CZ	2.35	0.45
5:E:45:VAL:HG13	10:J:28:ALA:CA	2.46	0.45
1:N:279:ARG:NH2	9:V:30:UNK:O	2.49	0.45
3:C:335:ILE:HD13	7:G:58:LEU:HD23	1.99	0.45
5:R:114:VAL:HG12	5:R:114:VAL:O	2.17	0.45
3:P:157:ILE:HD12	3:P:161:LEU:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:277:HIS:CD2	2:O:364:LEU:HB2	2.52	0.45
3:P:87:GLY:O	3:P:91:PHE:HB2	2.17	0.45
2:B:257:VAL:HG22	2:B:424:MET:HG3	1.98	0.45
5:R:86:ASN:ND2	5:R:148:ALA:HB2	2.32	0.45
2:O:73:SER:N	2:O:74:PRO:CD	2.80	0.45
2:O:259:THR:HG23	2:O:421:LYS:O	2.17	0.45
3:P:164:TRP:O	3:P:166:TRP:N	2.50	0.45
4:Q:68:VAL:HG12	4:Q:69:GLU:N	2.31	0.45
3:C:342:GLN:HB3	3:C:348:PHE:CE1	2.52	0.44
1:N:106:MET:HG3	1:N:203:ILE:HD13	1.99	0.44
3:C:285:ILE:HG21	3:C:290:GLY:HA3	1.97	0.44
1:N:43:ALA:HA	1:N:47:TYR:CD1	2.51	0.44
3:P:146:VAL:HG21	14:P:3001:3H1:C07	2.48	0.44
3:P:335:ILE:CD1	7:T:58:LEU:HD23	2.47	0.44
4:D:221:TYR:HD2	5:E:39:VAL:HG11	1.81	0.44
1:A:398:ARG:HH11	1:A:398:ARG:HG2	1.82	0.44
3:P:91:PHE:CE1	3:P:124:LEU:HD22	2.52	0.44
2:O:258:VAL:HG11	2:O:312:PHE:HD2	1.82	0.44
2:B:414:ALA:O	2:B:418:VAL:HG23	2.17	0.44
5:E:10:PHE:CD1	7:G:18:LEU:HD21	2.52	0.44
4:Q:108:ALA:HB1	17:Q:501:HEC:HMD1	1.98	0.44
7:G:74:PRO:O	7:G:76:ASP:N	2.51	0.44
3:C:164:TRP:O	3:C:165:ALA:C	2.56	0.44
1:A:250:VAL:HG21	1:A:325:VAL:CG1	2.47	0.44
3:P:338:TRP:CE2	7:T:59:TYR:HD1	2.35	0.44
2:O:287:ARG:HB3	9:V:53:GLU:HG3	1.98	0.44
6:S:99:ARG:HG2	6:S:99:ARG:HH11	1.82	0.44
6:S:21:TYR:C	6:S:21:TYR:CD2	2.91	0.44
2:B:227:ARG:NH1	2:B:228:SER:OG	2.50	0.44
4:Q:139:ALA:HB2	8:U:41:ASP:HA	1.99	0.44
5:E:171:ILE:CD1	5:E:176:ALA:HB3	2.48	0.44
2:O:305:GLN:HB3	2:O:306:PRO:CD	2.47	0.44
1:N:239:SER:HB2	7:T:17:SER:O	2.17	0.44
7:T:32:ASP:C	7:T:35:PRO:HD2	2.38	0.44
1:N:213:ARG:HG2	1:N:213:ARG:HH11	1.82	0.44
3:C:284:SER:HB2	3:C:285:ILE:HD12	2.00	0.44
2:O:59:THR:CG2	2:O:60:THR:N	2.76	0.44
2:O:344:LEU:HD23	2:O:417:PHE:CD2	2.51	0.44
3:C:164:TRP:O	3:C:167:GLY:N	2.51	0.44
1:A:136:GLN:NE2	9:I:50:LEU:CB	2.81	0.44
2:O:414:ALA:O	2:O:418:VAL:HG23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:68:LEU:HD23	2:O:186:ILE:HG21	1.98	0.44
4:D:220:TYR:O	4:D:224:ARG:HG2	2.17	0.44
8:U:23:HIS:O	8:U:26:GLN:HB2	2.17	0.44
2:B:181:TYR:CZ	2:B:182:ARG:HG3	2.52	0.44
2:B:27:THR:CG2	2:B:28:LYS:H	2.30	0.44
2:B:116:VAL:O	2:B:120:MET:HB2	2.17	0.44
2:B:265:GLY:O	2:B:266:SER:C	2.56	0.44
3:P:20:ILE:HG22	3:P:21:ASP:OD1	2.16	0.44
2:O:218:GLN:O	2:O:221:GLU:HG3	2.18	0.44
4:D:54:VAL:HG11	4:D:192:TRP:NE1	2.32	0.44
4:Q:223:LYS:C	4:Q:223:LYS:CD	2.84	0.44
8:U:52:GLU:C	8:U:53:GLN:HG3	2.38	0.44
5:E:95:PRO:HG3	3:P:263:LEU:HA	2.00	0.44
3:P:338:TRP:NE1	7:T:59:TYR:HE1	2.16	0.44
1:A:375:VAL:O	1:A:379:ILE:HD12	2.18	0.44
5:E:29:SER:OG	5:E:30:GLU:N	2.50	0.44
1:N:264:ASP:HA	1:N:265:PRO:HD3	1.79	0.44
3:C:139:MET:CE	3:C:270:LYS:H	2.29	0.44
7:T:30:PHE:O	7:T:35:PRO:HD3	2.18	0.44
4:D:68:VAL:HG12	4:D:69:GLU:N	2.32	0.44
3:P:344:VAL:HG12	3:P:349:ILE:HD11	1.99	0.44
2:O:26:ILE:HG23	2:O:26:ILE:O	2.17	0.44
3:P:19:LEU:HD13	14:P:3002:3H1:H25A	1.99	0.44
2:B:202:ALA:CB	2:B:229:GLY:H	2.30	0.44
4:Q:54:VAL:HG11	4:Q:192:TRP:CE2	2.52	0.44
1:A:79:VAL:O	1:A:82:MET:HG2	2.18	0.44
5:E:41:ALA:O	5:E:45:VAL:HG23	2.18	0.44
1:A:246:ASP:HA	1:A:427:PRO:HB3	1.99	0.44
3:C:91:PHE:CE1	3:C:124:LEU:HD22	2.52	0.44
1:N:276:ILE:HG12	1:N:357:ALA:HB2	2.00	0.44
14:P:3002:3H1:H18	14:P:3002:3H1:H16	1.83	0.43
2:O:282:GLY:HA2	2:O:283:PRO:HD2	1.78	0.43
3:P:70:THR:HA	3:P:74:VAL:HG23	1.99	0.43
3:P:285:ILE:HG21	3:P:290:GLY:HA3	2.00	0.43
3:C:117:GLY:O	3:C:120:LEU:HB2	2.18	0.43
5:R:38:LEU:HD13	10:W:14:PHE:HZ	1.83	0.43
2:O:31:ASN:ND2	2:O:31:ASN:N	2.66	0.43
5:E:166:ASP:OD1	5:E:168:SER:HB3	2.18	0.43
1:N:307:PHE:CD1	1:N:307:PHE:C	2.90	0.43
5:E:86:ASN:HD22	5:E:148:ALA:CB	2.31	0.43
2:B:348:ALA:HA	2:B:414:ALA:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:PHE:CE1	1:A:322:PHE:N	2.85	0.43
1:N:430:GLN:HG3	7:T:4:PHE:O	2.18	0.43
5:R:55:VAL:O	5:R:56:THR:C	2.55	0.43
5:R:126:ARG:O	5:R:182:VAL:HG11	2.18	0.43
5:E:49:TYR:CE1	10:J:32:GLU:HG3	2.52	0.43
1:N:121:ALA:O	1:N:122:LEU:HB2	2.17	0.43
3:C:283:ARG:NH2	3:C:342:GLN:O	2.43	0.43
8:H:20:ILE:HD12	8:H:73:LEU:HA	2.00	0.43
2:B:385:GLU:C	2:B:387:LEU:H	2.21	0.43
1:N:369:LEU:CD1	1:N:392:LEU:HD21	2.47	0.43
1:A:61:HIS:CE1	1:A:134:ILE:HG12	2.53	0.43
2:O:73:SER:N	2:O:74:PRO:HD2	2.34	0.43
2:O:277:HIS:CD2	2:O:364:LEU:HD13	2.52	0.43
5:R:38:LEU:HB2	10:W:14:PHE:CE1	2.51	0.43
1:A:206:LYS:O	1:A:209:VAL:CG1	2.66	0.43
1:N:191:LYS:C	1:N:195:MET:HE2	2.38	0.43
1:N:433:ASP:CG	1:N:435:ASN:HB2	2.38	0.43
3:P:183:HIS:O	3:P:187:PRO:CD	2.66	0.43
1:N:147:ASN:O	1:N:148:VAL:C	2.55	0.43
1:A:145:MET:HB3	1:A:252:HIS:CD2	2.53	0.43
3:C:342:GLN:NE2	3:C:343:PRO:HD2	2.30	0.43
4:D:197:GLU:O	4:D:199:ASP:N	2.51	0.43
3:P:22:LEU:HA	3:P:23:PRO:HD3	1.85	0.43
5:E:123:ASP:O	5:E:127:VAL:HG22	2.19	0.43
4:Q:102:ARG:NH1	4:Q:109:LEU:HB2	2.34	0.43
3:P:169:PHE:O	3:P:170:SER:HB3	2.19	0.43
3:P:134:LEU:HD12	13:P:501:HEM:C3D	2.54	0.43
1:A:85:HIS:HD2	2:B:284:LEU:HB3	1.82	0.43
5:E:193:VAL:HG22	5:E:194:VAL:N	2.32	0.43
5:R:186:GLN:NE2	5:R:188:VAL:HG12	2.28	0.43
5:R:78:LEU:HD22	5:R:132:TRP:CE3	2.52	0.43
4:D:20:ALA:HB1	4:D:199:ASP:OD2	2.18	0.43
1:N:371:GLY:O	1:N:375:VAL:HG23	2.19	0.43
2:B:71:LEU:HD11	2:B:144:LEU:HD23	2.00	0.43
4:D:48:PHE:CG	4:D:65:ALA:HB2	2.54	0.43
1:A:7:THR:HG21	2:B:113:ARG:NE	2.34	0.43
4:D:215:LEU:HD13	5:E:46:ALA:HB3	1.98	0.43
5:E:114:VAL:O	5:E:114:VAL:HG12	2.18	0.43
6:S:73:ARG:HD3	6:S:73:ARG:HA	1.65	0.43
1:N:219:VAL:HG12	1:N:220:SER:N	2.33	0.43
2:B:206:LEU:HG	2:B:206:LEU:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:132:PHE:CE1	2:B:191:LEU:HB3	2.52	0.43
1:N:203:ILE:HG22	1:N:204:SER:N	2.34	0.43
1:N:206:LYS:O	1:N:208:LEU:N	2.52	0.43
1:A:45:SER:HA	1:A:48:GLU:CG	2.48	0.43
3:C:243:LEU:HD21	3:C:251:LEU:HG	2.01	0.43
10:W:38:GLY:O	10:W:42:ILE:HG13	2.17	0.43
7:G:32:ASP:C	7:G:35:PRO:HD2	2.39	0.43
3:C:212:ILE:HD12	6:F:62:ILE:HG12	2.01	0.43
2:O:156:GLN:NE2	9:V:77:ARG:C	2.71	0.43
4:D:241:LYS:HA	4:D:241:LYS:CE	2.39	0.43
4:Q:10:PHE:CD2	8:U:74:PHE:CE2	3.07	0.43
7:T:72:LYS:HG2	8:U:56:GLU:OE2	2.18	0.43
1:A:39:VAL:O	1:A:39:VAL:HG13	2.19	0.43
7:G:41:PHE:CE2	7:G:45:VAL:HB	2.54	0.43
3:P:4:ASN:OD1	3:P:7:LYS:HD2	2.19	0.43
2:O:111:CYS:HB3	2:O:119:VAL:HG11	2.00	0.43
3:P:377:MET:HE2	6:S:20:TYR:HB2	2.01	0.43
5:R:152:ASP:C	5:R:153:PHE:CD1	2.92	0.43
1:A:373:THR:HB	1:A:374:PRO:CD	2.44	0.43
3:C:326:PHE:HA	3:C:367:PHE:HZ	1.83	0.43
4:D:197:GLU:O	4:D:198:HIS:C	2.57	0.43
2:B:144:LEU:CB	2:B:183:ILE:HD12	2.48	0.43
3:C:121:LEU:HG	3:C:125:MET:HE2	1.99	0.43
2:O:31:ASN:H	2:O:31:ASN:ND2	2.16	0.43
3:P:207:ASN:ND2	3:P:314:ARG:NH1	2.66	0.43
3:C:263:LEU:HD23	5:R:95:PRO:HG3	2.01	0.43
5:E:170:ARG:HA	5:E:179:ASN:HB3	2.00	0.43
3:C:219:ILE:HB	3:C:224:TYR:HD1	1.83	0.43
2:O:305:GLN:HB3	2:O:306:PRO:HD2	2.01	0.43
7:T:34:LEU:N	7:T:35:PRO:CD	2.81	0.43
2:B:272:PHE:O	2:B:276:GLN:N	2.52	0.43
2:O:29:LEU:HB3	2:O:30:PRO:CD	2.46	0.43
2:B:189:GLU:O	2:B:190:GLN:C	2.57	0.43
8:H:15:ASP:O	8:H:17:LEU:N	2.51	0.43
2:B:24:LEU:O	2:B:24:LEU:HG	2.19	0.43
1:A:223:TYR:CD2	1:A:223:TYR:N	2.87	0.43
2:O:408:ALA:O	2:O:411:VAL:N	2.51	0.43
5:E:69:LEU:H	5:E:69:LEU:HG	1.59	0.43
3:P:186:LEU:HB2	3:P:187:PRO:HD3	2.01	0.43
3:P:333:LEU:HD21	3:P:359:TYR:CE1	2.54	0.43
5:E:166:ASP:OD2	5:E:170:ARG:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:227:TRP:O	4:Q:228:SER:C	2.56	0.43
3:P:58:ALA:O	3:P:177:THR:HG22	2.19	0.43
1:N:20:ASP:N	1:N:20:ASP:OD2	2.50	0.43
1:A:281:ASP:OD2	1:A:284:PHE:CE1	2.71	0.43
8:U:50:THR:OG1	8:U:51:GLU:N	2.50	0.43
4:D:130:LEU:HD11	4:D:158:ILE:HD12	2.01	0.43
4:Q:147:LEU:HD13	4:Q:157:ALA:HB1	2.01	0.43
3:P:172:ASP:OD1	3:P:173:ASN:N	2.42	0.43
5:E:153:PHE:CE2	5:E:172:ARG:HB3	2.54	0.43
10:W:17:THR:HG22	10:W:17:THR:O	2.17	0.43
3:C:198:LEU:HD23	3:C:198:LEU:HA	1.77	0.43
2:O:206:LEU:O	2:O:206:LEU:HG	2.18	0.43
2:O:285:ILE:O	2:O:288:GLY:N	2.51	0.43
1:N:388:ARG:HD3	1:N:388:ARG:H	1.84	0.43
2:O:135:TRP:O	2:O:136:GLU:C	2.57	0.43
3:P:326:PHE:O	3:P:329:LEU:HB3	2.19	0.43
6:S:32:MET:HE1	6:S:87:LYS:H	1.83	0.43
2:O:150:VAL:O	2:O:153:GLN:HB2	2.19	0.43
1:A:191:LYS:C	1:A:195:MET:HE2	2.39	0.43
3:C:263:LEU:HA	5:R:95:PRO:HG3	2.00	0.43
2:B:50:PHE:HD2	2:B:104:LYS:HZ1	1.67	0.43
4:D:105:ASN:O	4:D:106:ASN:HB2	2.19	0.43
2:O:241:GLY:HA2	2:O:423:SER:OG	2.19	0.43
8:U:27:THR:CG2	8:U:28:GLU:N	2.82	0.43
6:F:21:TYR:C	6:F:21:TYR:CD2	2.92	0.43
2:B:38:LEU:O	2:B:38:LEU:HG	2.18	0.43
6:F:73:ARG:HA	6:F:73:ARG:HD3	1.67	0.43
2:O:394:ALA:C	2:O:396:SER:H	2.22	0.43
3:P:157:ILE:HD12	3:P:161:LEU:CD1	2.49	0.42
2:B:385:GLU:CD	2:B:392:HIS:HA	2.40	0.42
2:B:258:VAL:HG11	2:B:312:PHE:HD2	1.83	0.42
8:H:40:CYS:O	8:H:44:VAL:HG23	2.18	0.42
7:G:34:LEU:N	7:G:35:PRO:CD	2.81	0.42
5:R:153:PHE:CE2	5:R:172:ARG:HB3	2.54	0.42
1:A:294:LEU:HB2	1:A:341:GLU:HG3	2.01	0.42
7:T:53:LEU:O	7:T:56:TYR:HB3	2.19	0.42
2:B:58:GLU:OE2	2:B:66:ALA:HB3	2.19	0.42
1:N:274:ASN:HA	1:N:274:ASN:HD22	1.65	0.42
7:G:68:ARG:HH11	7:G:68:ARG:HG2	1.83	0.42
3:P:157:ILE:O	3:P:159:HIS:N	2.52	0.42
2:B:31:ASN:HB2	2:B:201:SER:OG	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:285:ILE:O	2:B:288:GLY:N	2.52	0.42
2:O:24:LEU:HG	2:O:24:LEU:O	2.19	0.42
9:V:72:ALA:HB1	9:V:73:PRO:CD	2.49	0.42
2:O:327:ILE:HG22	9:V:55:MET:CE	2.48	0.42
10:J:58:LYS:HB2	10:J:59:TYR:CE1	2.54	0.42
2:B:394:ALA:C	2:B:396:SER:N	2.72	0.42
2:B:111:CYS:HB3	2:B:119:VAL:HG11	2.01	0.42
2:B:282:GLY:HA2	2:B:283:PRO:HD2	1.78	0.42
2:B:52:LYS:O	2:B:203:ARG:NH2	2.51	0.42
3:P:70:THR:HA	3:P:74:VAL:CG2	2.49	0.42
2:B:295:LEU:HA	2:B:343:GLN:HG2	2.02	0.42
5:E:78:LEU:HD22	5:E:132:TRP:CE3	2.53	0.42
4:D:227:TRP:O	4:D:228:SER:C	2.57	0.42
3:C:98:HIS:CD2	13:C:502:HEM:NC	2.87	0.42
2:B:291:VAL:C	2:B:293:SER:H	2.23	0.42
1:N:39:VAL:HG13	1:N:39:VAL:O	2.19	0.42
3:C:156:TYR:C	3:C:158:GLY:N	2.71	0.42
2:B:259:THR:HG23	2:B:421:LYS:O	2.19	0.42
4:D:218:LEU:HD11	5:E:42:THR:HG22	2.01	0.42
7:T:28:ASN:HB2	7:T:32:ASP:HB3	2.01	0.42
1:A:264:ASP:HA	1:A:265:PRO:HD3	1.81	0.42
4:Q:91:PHE:HA	4:Q:92:PRO:HD3	1.84	0.42
3:C:231:LEU:O	3:C:235:LEU:HG	2.19	0.42
2:B:327:ILE:CD1	9:I:58:ARG:HB2	2.49	0.42
6:F:31:LEU:HD21	6:F:65:ALA:HB2	2.02	0.42
5:E:152:ASP:C	5:E:153:PHE:CD1	2.92	0.42
3:C:344:VAL:HG12	3:C:349:ILE:HD11	2.01	0.42
5:E:118:ARG:HE	5:E:118:ARG:HB2	1.67	0.42
10:J:25:VAL:O	10:J:29:VAL:HG23	2.19	0.42
1:N:109:VAL:HA	1:N:112:LEU:HD12	2.02	0.42
4:Q:10:PHE:CD1	4:Q:10:PHE:N	2.88	0.42
6:F:28:LYS:HE3	6:F:80:TRP:CH2	2.55	0.42
4:D:14:HIS:HB3	4:D:21:LEU:HA	2.01	0.42
2:O:287:ARG:CB	9:V:53:GLU:HG3	2.49	0.42
1:N:262:TRP:O	1:N:386:TYR:HE1	2.02	0.42
5:E:136:VAL:HG12	5:E:138:VAL:HG23	2.01	0.42
2:O:207:VAL:HG12	2:O:208:GLY:N	2.27	0.42
2:O:207:VAL:O	2:O:216:LEU:HD21	2.18	0.42
7:T:29:ILE:CD1	7:T:29:ILE:H	2.12	0.42
1:A:371:GLY:O	1:A:375:VAL:HG23	2.20	0.42
1:A:102:LEU:H	1:A:102:LEU:HG	1.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:LEU:HD12	1:A:105:ASP:OD2	2.19	0.42
1:N:85:HIS:HD2	2:O:284:LEU:HB3	1.85	0.42
2:O:248:ASN:HD21	2:O:250:HIS:HB3	1.85	0.42
5:R:40:THR:HG21	11:R:3005:PEE:O2P	2.19	0.42
3:P:193:ILE:O	3:P:194:THR:C	2.58	0.42
3:P:333:LEU:HA	3:P:336:LEU:HD12	2.02	0.42
3:C:333:LEU:HA	3:C:336:LEU:HD12	2.00	0.42
1:A:4:TYR:O	1:A:5:ALA:C	2.58	0.42
2:B:330:ALA:O	2:B:432:SER:HB2	2.19	0.42
1:A:439:SER:HA	1:A:442:TYR:CE2	2.54	0.42
1:A:350:THR:OG1	1:A:353:GLU:HG3	2.19	0.42
3:C:14:MET:O	3:C:18:SER:OG	2.31	0.42
3:P:90:PHE:HB3	3:P:236:MET:CE	2.50	0.42
4:Q:162:PRO:HA	4:Q:163:PRO:HD2	1.85	0.42
2:B:147:ASP:O	2:B:150:VAL:HG22	2.19	0.42
7:G:81:GLN:OXT	8:H:49:HIS:N	2.52	0.42
4:D:75:ASP:OD2	4:D:79:GLU:HB2	2.20	0.42
3:P:28:ILE:HG13	3:P:225:TYR:CE2	2.54	0.42
6:S:42:ASP:OD2	6:S:101:ARG:NH1	2.51	0.42
3:P:350:ILE:HA	3:P:350:ILE:HD12	1.90	0.42
2:O:59:THR:CG2	2:O:60:THR:H	2.32	0.42
1:A:6:GLN:C	1:A:8:LEU:N	2.72	0.42
1:N:332:ASP:HB2	1:N:430:GLN:HG2	2.00	0.42
1:A:147:ASN:O	1:A:148:VAL:C	2.57	0.42
6:S:26:PHE:CE1	6:S:33:ARG:HA	2.55	0.42
5:E:91:TRP:CH2	5:E:92:ARG:HD2	2.54	0.42
6:F:52:LYS:NZ	7:G:11:ARG:HD3	2.35	0.42
1:N:106:MET:HB3	1:N:107:PRO:CD	2.50	0.42
5:R:29:SER:OG	5:R:30:GLU:N	2.53	0.42
3:P:106:GLY:HA2	3:P:108:TYR:CZ	2.55	0.42
2:O:52:LYS:O	2:O:203:ARG:NH2	2.53	0.42
2:O:306:PRO:HB3	9:V:52:ARG:N	2.35	0.42
10:W:16:ARG:HB2	10:W:19:THR:OG1	2.19	0.42
1:N:350:THR:OG1	1:N:353:GLU:HG3	2.19	0.42
1:N:170:THR:HG22	1:N:172:GLU:H	1.83	0.42
1:A:114:ALA:CB	1:A:216:PHE:CE2	3.03	0.42
2:B:189:GLU:O	2:B:191:LEU:N	2.53	0.42
1:N:255:LEU:O	1:N:321:GLY:HA3	2.20	0.42
1:N:180:ALA:O	1:N:183:ALA:HB3	2.20	0.42
2:B:71:LEU:CD1	2:B:144:LEU:HD23	2.50	0.42
3:P:358:SER:O	3:P:362:ILE:HG13	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:155:PRO:O	3:P:156:TYR:CB	2.67	0.42
9:V:61:ARG:C	9:V:62:ARG:CG	2.88	0.42
4:Q:16:GLY:HA3	4:Q:19:SER:OG	2.20	0.42
4:D:234:LYS:HZ1	5:E:13:TYR:HE2	1.68	0.42
2:B:56:ARG:HE	2:B:171:ALA:HB1	1.85	0.42
1:N:398:ARG:HG2	1:N:398:ARG:NH1	2.35	0.42
2:B:161:GLU:HA	2:B:161:GLU:OE1	2.20	0.42
1:N:63:ALA:O	1:N:116:VAL:CG1	2.68	0.41
4:Q:10:PHE:CD2	8:U:74:PHE:HE2	2.37	0.41
5:R:78:LEU:HB3	5:R:132:TRP:CH2	2.55	0.41
3:P:346:HIS:CG	3:P:347:PRO:HA	2.55	0.41
3:C:350:ILE:HA	3:C:350:ILE:HD12	1.90	0.41
5:E:64:ALA:HA	3:P:167:GLY:O	2.20	0.41
10:W:42:ILE:O	10:W:46:LEU:HG	2.20	0.41
4:Q:110:PRO:HA	4:Q:111:PRO:HD2	1.91	0.41
3:C:327:TRP:CE2	7:G:48:VAL:HG22	2.56	0.41
1:A:37:VAL:HG22	1:A:109:VAL:HG11	2.02	0.41
8:H:73:LEU:HD12	8:H:73:LEU:C	2.41	0.41
3:P:88:ALA:O	3:P:92:PHE:HD1	2.03	0.41
6:S:16:ILE:O	6:S:19:TRP:HB3	2.20	0.41
2:B:277:HIS:CD2	2:B:364:LEU:HD13	2.55	0.41
1:A:4:TYR:CZ	1:A:8:LEU:HD11	2.55	0.41
3:P:182:LEU:HA	3:P:182:LEU:HD13	1.88	0.41
6:F:102:LEU:HA	6:F:102:LEU:HD23	1.88	0.41
2:B:158:GLY:O	2:B:162:ASN:ND2	2.53	0.41
7:T:45:VAL:HG22	7:T:45:VAL:O	2.20	0.41
3:P:105:TYR:HA	3:P:315:THR:HG22	2.01	0.41
5:E:186:GLN:NE2	5:E:188:VAL:HG12	2.36	0.41
1:A:147:ASN:C	1:A:149:THR:N	2.73	0.41
4:D:95:TYR:CD2	4:D:101:ALA:HA	2.54	0.41
3:P:34:PHE:HB2	20:P:381:HOH:O	2.20	0.41
1:N:394:GLU:O	1:N:395:TRP:C	2.58	0.41
2:O:132:PHE:CE1	2:O:191:LEU:HB3	2.56	0.41
1:A:231:LEU:CD2	1:A:232:PRO:HD2	2.46	0.41
5:R:49:TYR:CD1	10:W:32:GLU:HG3	2.55	0.41
3:C:319:ARG:NH1	3:C:322:SER:OG	2.53	0.41
5:E:164:HIS:HD2	5:E:173:LYS:HD3	1.84	0.41
3:C:70:THR:HA	3:C:74:VAL:HG23	2.02	0.41
3:P:186:LEU:HA	3:P:186:LEU:HD23	1.72	0.41
8:U:13:LEU:HD23	8:U:13:LEU:N	2.34	0.41
8:U:58:LEU:HD12	8:U:58:LEU:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:42:SER:O	2:B:113:ARG:HD2	2.20	0.41
1:N:351:GLU:O	1:N:354:VAL:HG22	2.21	0.41
1:N:424:ALA:HB1	1:N:428:ILE:HG21	2.02	0.41
3:P:313:GLN:NE2	6:S:36:THR:OG1	2.51	0.41
2:O:376:GLN:NE2	9:V:77:ARG:HH22	2.12	0.41
3:P:200:PHE:O	3:P:201:LEU:C	2.58	0.41
1:N:106:MET:HB3	1:N:107:PRO:HD3	2.02	0.41
5:E:187:PHE:CD1	5:E:193:VAL:HB	2.54	0.41
7:T:29:ILE:CD1	7:T:29:ILE:N	2.80	0.41
1:N:371:GLY:C	1:N:374:PRO:HD2	2.41	0.41
2:B:166:ALA:HB2	2:B:244:ILE:HG13	2.03	0.41
2:O:417:PHE:CD2	2:O:417:PHE:C	2.94	0.41
4:D:165:TYR:O	4:D:168:ILE:HB	2.20	0.41
3:C:212:ILE:HD12	6:F:62:ILE:HG23	2.01	0.41
9:I:67:GLY:O	9:I:68:ILE:HD13	2.21	0.41
8:H:27:THR:CG2	8:H:28:GLU:N	2.82	0.41
2:O:385:GLU:C	2:O:387:LEU:H	2.23	0.41
2:B:76:THR:HG23	2:B:82:SER:HB2	2.01	0.41
3:P:201:LEU:HD23	14:P:3002:3H1:CL12	2.57	0.41
4:Q:197:GLU:O	4:Q:198:HIS:C	2.59	0.41
3:C:92:PHE:HA	3:C:95:ILE:HG22	2.02	0.41
2:B:166:ALA:HA	2:B:240:TRP:CZ3	2.56	0.41
4:Q:134:TYR:OH	4:Q:160:MET:O	2.27	0.41
4:Q:102:ARG:HH11	4:Q:102:ARG:HG2	1.84	0.41
3:P:220:PRO:O	3:P:221:PHE:C	2.57	0.41
5:E:157:TYR:CE1	5:E:162:GLY:HA2	2.55	0.41
1:A:78:GLU:OE1	1:A:108:LYS:HE3	2.21	0.41
9:V:49:LEU:O	9:V:50:LEU:HD23	2.20	0.41
3:C:285:ILE:HB	3:C:291:GLY:HA2	2.02	0.41
3:C:32:TRP:NE1	13:C:502:HEM:O2D	2.51	0.41
2:B:73:SER:N	2:B:74:PRO:HD2	2.35	0.41
3:P:326:PHE:HA	3:P:367:PHE:HZ	1.85	0.41
2:O:279:LEU:HD13	2:O:344:LEU:HD11	2.03	0.41
2:O:272:PHE:O	2:O:276:GLN:N	2.53	0.41
1:N:156:THR:HA	1:N:159:GLN:HB3	2.02	0.41
3:P:242:THR:CA	4:Q:208:MET:HE1	2.50	0.41
5:E:105:GLU:O	5:E:107:ASN:N	2.54	0.41
3:P:230:ILE:O	3:P:233:LEU:HB3	2.20	0.41
5:R:105:GLU:O	5:R:107:ASN:N	2.53	0.41
1:A:307:PHE:HA	1:A:323:HIS:O	2.20	0.41
4:D:194:ALA:O	4:D:195:GLU:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:200:PHE:O	3:C:201:LEU:C	2.58	0.41
5:R:113:ASP:C	5:R:115:SER:H	2.23	0.41
1:A:106:MET:N	1:A:107:PRO:HD2	2.36	0.41
3:C:38:LEU:HD23	3:C:38:LEU:HA	1.88	0.41
2:B:73:SER:N	2:B:74:PRO:CD	2.84	0.41
5:R:171:ILE:HD13	5:R:176:ALA:HB3	2.02	0.41
1:A:4:TYR:O	1:A:6:GLN:N	2.54	0.41
4:Q:142:VAL:O	4:Q:142:VAL:HG23	2.20	0.41
2:O:227:ARG:HG3	2:O:228:SER:N	2.36	0.41
3:P:270:LYS:CD	3:P:279:TYR:HE2	2.34	0.41
1:A:382:HIS:CE1	1:A:390:ILE:HB	2.56	0.41
2:B:51:ILE:HG22	2:B:52:LYS:N	2.36	0.41
3:C:134:LEU:HD12	13:C:501:HEM:C3D	2.56	0.41
5:E:185:TYR:HB3	5:E:195:VAL:HA	2.03	0.41
1:A:182:LEU:HD23	1:A:182:LEU:N	2.35	0.41
7:T:72:LYS:NZ	8:U:52:GLU:OE1	2.46	0.41
3:P:350:ILE:HG23	3:P:351:ILE:N	2.36	0.41
8:H:17:LEU:CD1	8:H:73:LEU:HD22	2.51	0.41
5:R:47:THR:HG21	11:R:3005:PEE:H23	2.03	0.41
1:N:62:LEU:HD11	1:N:127:ILE:HG12	2.02	0.41
5:R:170:ARG:HA	5:R:179:ASN:HB3	2.03	0.41
2:O:279:LEU:CD2	2:O:344:LEU:HD12	2.51	0.41
2:B:259:THR:CG2	2:B:260:GLU:N	2.84	0.41
1:A:191:LYS:N	1:A:195:MET:HE2	2.36	0.41
1:A:6:GLN:O	1:A:8:LEU:N	2.53	0.41
7:G:30:PHE:O	7:G:35:PRO:HD3	2.20	0.41
2:B:235:ALA:O	2:B:236:LYS:C	2.58	0.41
1:N:250:VAL:HG21	1:N:325:VAL:CG1	2.51	0.41
2:B:337:ILE:HD12	2:B:434:PRO:HD2	2.02	0.41
1:N:163:LEU:HA	1:N:163:LEU:HD23	1.94	0.41
3:C:52:LEU:HD13	13:C:501:HEM:O2D	2.21	0.41
8:U:20:ILE:HD12	8:U:73:LEU:HA	2.03	0.41
4:Q:21:LEU:HD13	4:Q:192:TRP:HB2	2.03	0.41
1:A:369:LEU:HB3	1:A:375:VAL:HG22	2.03	0.41
3:C:284:SER:O	3:C:286:PRO:HD3	2.21	0.41
7:G:74:PRO:C	7:G:76:ASP:H	2.25	0.41
2:O:144:LEU:CB	2:O:183:ILE:HD12	2.49	0.41
4:D:228:SER:O	4:D:229:VAL:C	2.58	0.41
3:C:38:LEU:HB3	13:C:502:HEM:HMB1	2.03	0.41
3:C:40:VAL:HG11	3:C:233:LEU:HD11	2.02	0.41
2:B:169:LYS:O	2:B:170:THR:CG2	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:89:TYR:CE1	6:S:90:LEU:HB2	2.56	0.41
1:A:2:ALA:HB3	2:B:113:ARG:HH21	1.87	0.41
2:B:42:SER:OG	2:B:43:PRO:HD2	2.21	0.41
1:N:294:LEU:HD11	1:N:334:MET:HE3	2.02	0.41
1:A:294:LEU:HD11	1:A:334:MET:CE	2.50	0.41
4:D:110:PRO:HA	4:D:111:PRO:HD2	1.88	0.41
3:P:305:ILE:HB	3:P:306:PRO:HD3	2.03	0.41
4:D:70:VAL:O	4:D:83:ARG:HG2	2.21	0.41
1:N:361:LEU:HD23	1:N:399:ILE:HD13	2.03	0.41
4:Q:232:SER:HB3	7:T:23:GLN:HE22	1.85	0.41
3:P:192:GLY:O	3:P:195:ILE:HB	2.21	0.41
1:A:388:ARG:HG2	1:A:389:ARG:N	2.36	0.40
1:A:82:MET:HE3	1:A:105:ASP:HB3	2.02	0.40
1:A:106:MET:HB3	1:A:107:PRO:HD3	2.03	0.40
2:O:293:SER:OG	2:O:296:TYR:HB2	2.21	0.40
9:I:49:LEU:HB3	9:I:55:MET:HG3	2.02	0.40
3:C:164:TRP:O	3:C:166:TRP:N	2.54	0.40
3:P:104:TYR:CD2	11:P:3007:PEE:H14	2.56	0.40
4:Q:220:TYR:O	4:Q:224:ARG:HG2	2.20	0.40
2:B:62:ASN:CB	2:B:190:GLN:HE21	2.34	0.40
2:O:215:ASP:O	2:O:216:LEU:C	2.59	0.40
7:T:72:LYS:HE2	8:U:57:GLU:OE1	2.22	0.40
1:A:233:ARG:NH1	1:A:233:ARG:CG	2.84	0.40
1:N:89:TYR:O	1:N:95:THR:HG23	2.21	0.40
7:T:73:ASN:HA	7:T:74:PRO:HD2	1.97	0.40
6:S:70:LEU:O	6:S:70:LEU:HD12	2.20	0.40
1:N:295:ALA:O	1:N:299:VAL:HG23	2.21	0.40
5:R:24:SER:OG	5:R:26:GLN:HB2	2.22	0.40
2:B:141:GLN:N	2:B:142:PRO:CD	2.84	0.40
1:A:332:ASP:HB2	1:A:430:GLN:HG2	2.03	0.40
1:A:351:GLU:HA	1:A:354:VAL:HG22	2.03	0.40
1:A:351:GLU:O	1:A:354:VAL:HG22	2.21	0.40
2:O:169:LYS:HD2	2:O:238:THR:HG21	2.03	0.40
6:S:53:ASP:OD1	6:S:54:LEU:N	2.55	0.40
4:Q:145:GLU:HG2	4:Q:146:GLY:N	2.35	0.40
2:O:366:ALA:C	2:O:370:MET:HE2	2.41	0.40
3:P:284:SER:O	3:P:286:PRO:HD3	2.21	0.40
3:C:19:LEU:HD13	14:C:2002:3H1:H25A	2.04	0.40
3:P:157:ILE:CG1	3:P:158:GLY:N	2.69	0.40
10:J:10:TYR:HE2	10:J:15:ARG:HD2	1.79	0.40
6:F:49:ARG:HD3	2:O:135:TRP:CE2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:235:LEU:HA	3:C:235:LEU:HD23	1.88	0.40
5:R:77:LYS:HE2	5:R:79:SER:OG	2.22	0.40
5:R:165:TYR:HA	5:R:170:ARG:O	2.22	0.40
2:B:317:SER:OG	2:B:318:ASP:N	2.54	0.40
3:C:219:ILE:HB	3:C:220:PRO:HD2	2.04	0.40
1:N:351:GLU:OE2	1:N:404:ALA:CB	2.69	0.40
5:E:31:ASP:O	5:E:32:ARG:C	2.57	0.40
2:O:235:ALA:O	2:O:236:LYS:C	2.60	0.40
3:C:109:LEU:HA	3:C:109:LEU:HD23	1.76	0.40
4:D:47:ALA:HB1	4:D:89:ASP:O	2.22	0.40
2:B:353:THR:HG22	2:B:354:GLU:N	2.35	0.40
2:B:209:ILE:HG13	2:B:379:LEU:HD13	2.02	0.40
2:O:33:LEU:HD12	2:O:204:MET:O	2.21	0.40
1:A:19:LEU:HD23	1:A:19:LEU:N	2.36	0.40
2:B:135:TRP:O	2:B:136:GLU:C	2.60	0.40
5:R:106:ILE:HG22	5:R:106:ILE:O	2.21	0.40
1:A:4:TYR:HB3	2:B:114:ASP:OD2	2.20	0.40
1:N:402:VAL:HG12	1:N:403:ASP:N	2.37	0.40
6:F:26:PHE:CE1	6:F:33:ARG:HA	2.56	0.40
5:E:24:SER:OG	5:E:26:GLN:HB2	2.22	0.40
7:G:48:VAL:O	7:G:51:PRO:HD2	2.22	0.40
1:A:109:VAL:O	1:A:112:LEU:N	2.54	0.40
2:O:24:LEU:HD21	2:O:392:HIS:CD2	2.56	0.40
3:C:243:LEU:HD12	3:C:243:LEU:HA	1.90	0.40
1:N:432:LEU:HG	1:N:433:ASP:H	1.85	0.40
2:O:306:PRO:HA	9:V:52:ARG:HG3	2.03	0.40
8:H:27:THR:HG22	8:H:28:GLU:N	2.36	0.40
1:N:248:LEU:HB3	1:N:249:PRO:HD2	2.03	0.40
7:T:68:ARG:HH11	7:T:68:ARG:HG2	1.85	0.40
3:C:186:LEU:HA	3:C:186:LEU:HD23	1.75	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	441/446 (99%)	383 (87%)	47 (11%)	11 (2%)	7 41
1	N	440/446 (99%)	382 (87%)	45 (10%)	13 (3%)	5 36
2	B	419/441 (95%)	323 (77%)	73 (17%)	23 (6%)	2 18
2	O	420/441 (95%)	331 (79%)	67 (16%)	22 (5%)	2 19
3	C	378/380 (100%)	333 (88%)	33 (9%)	12 (3%)	5 33
3	P	377/380 (99%)	329 (87%)	36 (10%)	12 (3%)	5 33
4	D	239/241 (99%)	204 (85%)	32 (13%)	3 (1%)	15 58
4	Q	239/241 (99%)	201 (84%)	35 (15%)	3 (1%)	15 58
5	E	194/196 (99%)	153 (79%)	26 (13%)	15 (8%)	1 8
5	R	194/196 (99%)	153 (79%)	27 (14%)	14 (7%)	1 10
6	F	99/110 (90%)	90 (91%)	8 (8%)	1 (1%)	19 64
6	S	99/110 (90%)	88 (89%)	8 (8%)	3 (3%)	5 36
7	G	79/81 (98%)	64 (81%)	10 (13%)	5 (6%)	2 13
7	T	77/81 (95%)	63 (82%)	10 (13%)	4 (5%)	2 19
8	H	68/77 (88%)	59 (87%)	7 (10%)	2 (3%)	6 36
8	U	65/77 (84%)	53 (82%)	12 (18%)	0	100 100
9	I	29/47 (62%)	23 (79%)	4 (14%)	2 (7%)	1 11
9	V	29/47 (62%)	21 (72%)	5 (17%)	3 (10%)	1 4
10	J	59/61 (97%)	51 (86%)	5 (8%)	3 (5%)	2 20
10	W	57/61 (93%)	45 (79%)	10 (18%)	2 (4%)	4 31
All	All	4002/4160 (96%)	3349 (84%)	500 (12%)	153 (4%)	4 28

All (153) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	94	GLN
1	A	282	ARG
2	B	20	GLY
2	B	26	ILE
2	B	29	LEU
2	B	171	ALA
2	B	226	ILE
2	B	230	ALA

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Mol	Chain	Res	Type
3	C	20	ILE
4	D	198	HIS
5	E	69	LEU
5	E	70	ALA
6	F	77	LYS
7	G	7	LEU
1	N	282	ARG
1	N	433	ASP
2	O	26	ILE
2	O	171	ALA
2	O	226	ILE
2	O	230	ALA
3	P	20	ILE
4	Q	198	HIS
5	R	69	LEU
5	R	70	ALA
6	S	77	LYS
7	T	7	LEU
10	W	60	GLU
1	A	5	ALA
1	A	72	CYS
1	A	433	ASP
2	B	22	GLU
2	B	38	LEU
2	B	63	LEU
2	B	207	VAL
2	B	282	GLY
2	B	389	SER
3	C	19	LEU
3	C	58	ALA
3	C	202	HIS
5	E	72	SER
5	E	123	ASP
5	E	188	VAL
7	G	75	ALA
9	I	60	ALA
10	J	56	LYS
1	N	72	CYS
1	N	94	GLN
1	N	207	GLU
1	N	262	TRP
2	O	19	PRO

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Mol	Chain	Res	Type
2	O	63	LEU
2	O	164	HIS
2	O	282	GLY
2	O	389	SER
3	P	19	LEU
3	P	111	LYS
3	P	158	GLY
3	P	165	ALA
3	P	170	SER
3	P	202	HIS
5	R	8	PRO
5	R	63	SER
5	R	72	SER
5	R	113	ASP
7	T	75	ALA
10	W	56	LYS
1	A	404	ALA
2	B	31	ASN
2	B	266	SER
2	B	283	PRO
2	B	386	ALA
3	C	156	TYR
3	C	165	ALA
5	E	63	SER
5	E	95	PRO
5	E	113	ASP
8	H	10	GLU
10	J	17	THR
1	N	159	GLN
2	O	38	LEU
2	O	207	VAL
2	O	283	PRO
3	P	156	TYR
3	P	379	ASN
5	R	21	ALA
5	R	123	ASP
5	R	130	PRO
6	S	11	ARG
7	T	33	ALA
1	A	3	THR
1	A	71	PRO
1	A	155	ALA

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Mol	Chain	Res	Type
1	A	262	TRP
2	B	30	PRO
2	B	152	PHE
2	B	250	HIS
2	B	290	SER
2	B	392	HIS
3	C	111	LYS
3	C	170	SER
5	E	8	PRO
5	E	130	PRO
5	E	141	HIS
8	H	49	HIS
1	N	206	LYS
1	N	288	LYS
1	N	404	ALA
1	N	428	ILE
2	O	201	SER
2	O	265	GLY
2	O	268	GLU
3	P	3	PRO
3	P	288	LYS
5	R	95	PRO
6	S	83	TYR
9	V	62	ARG
2	B	110	GLU
3	C	3	PRO
3	C	379	ASN
7	G	50	PRO
7	G	61	TRP
1	N	20	ASP
2	O	55	SER
2	O	236	LYS
2	O	250	HIS
2	O	290	SER
2	O	386	ALA
2	O	392	HIS
3	P	157	ILE
5	R	106	ILE
5	R	141	HIS
5	R	183	PRO
7	T	50	PRO
1	A	428	ILE

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Mol	Chain	Res	Type
2	B	236	LYS
3	C	366	LEU
4	D	176	PRO
5	E	106	ILE
5	E	177	PRO
7	G	33	ALA
9	I	62	ARG
10	J	32	GLU
1	N	71	PRO
4	Q	162	PRO
4	Q	176	PRO
9	V	60	ALA
5	E	137	GLY
5	R	177	PRO
3	C	157	ILE
4	D	162	PRO
9	V	48	PRO
2	O	29	LEU
5	E	74	ILE

5.3.2 Protein sidechains (i)

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%)	348 (95%)	17 (5%)	32	72
1	N	365/368 (99%)	347 (95%)	18 (5%)	31	72
2	B	332/347 (96%)	323 (97%)	9 (3%)	52	84
2	O	333/347 (96%)	324 (97%)	9 (3%)	52	84
3	C	329/329 (100%)	321 (98%)	8 (2%)	57	86
3	P	328/329 (100%)	315 (96%)	13 (4%)	38	76
4	D	200/200 (100%)	194 (97%)	6 (3%)	48	82
4	Q	200/200 (100%)	196 (98%)	4 (2%)	63	88
5	E	166/166 (100%)	159 (96%)	7 (4%)	36	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	R	166/166 (100%)	159 (96%)	7 (4%)	36	75
6	F	93/96 (97%)	89 (96%)	4 (4%)	35	74
6	S	93/96 (97%)	90 (97%)	3 (3%)	46	80
7	G	71/71 (100%)	65 (92%)	6 (8%)	13	47
7	T	69/71 (97%)	63 (91%)	6 (9%)	13	45
8	H	65/71 (92%)	62 (95%)	3 (5%)	33	73
8	U	63/71 (89%)	61 (97%)	2 (3%)	46	80
9	I	23/26 (88%)	22 (96%)	1 (4%)	35	74
9	V	23/26 (88%)	23 (100%)	0	100	100
10	J	49/49 (100%)	46 (94%)	3 (6%)	23	64
10	W	47/49 (96%)	44 (94%)	3 (6%)	22	62
All	All	3380/3446 (98%)	3251 (96%)	129 (4%)	40	77

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	THR
1	A	49	ASN
1	A	58	PHE
1	A	86	PHE
1	A	87	ASN
1	A	106	MET
1	A	184	SER
1	A	223	TYR
1	A	226	ASP
1	A	281	ASP
1	A	307	PHE
1	A	342	TRP
1	A	388	ARG
1	A	395	TRP
1	A	431	LEU
1	A	432	LEU
1	A	443	TRP
2	B	31	ASN
2	B	102	ARG
2	B	124	LEU
2	B	154	SER
2	B	160	LEU

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Mol	Chain	Res	Type
2	B	227	ARG
2	B	248	ASN
2	B	296	TYR
2	B	403	ASP
3	C	21	ASP
3	C	81	ARG
3	C	91	PHE
3	C	149	ASN
3	C	182	LEU
3	C	213	SER
3	C	234	THR
3	C	236	MET
4	D	2	GLU
4	D	43	MET
4	D	169	LEU
4	D	173	ASP
4	D	240	PRO
4	D	241	LYS
5	E	6	THR
5	E	52	LYS
5	E	59	ILE
5	E	65	SER
5	E	69	LEU
5	E	80	ASP
5	E	135	LEU
6	F	63	LYS
6	F	70	LEU
6	F	84	GLU
6	F	91	GLU
7	G	4	PHE
7	G	15	THR
7	G	16	TYR
7	G	29	ILE
7	G	41	PHE
7	G	63	THR
8	H	10	GLU
8	H	48	SER
8	H	71	HIS
9	I	71	ASN
10	J	11	SER
10	J	22	LEU
10	J	59	TYR

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Mol	Chain	Res	Type
1	N	3	THR
1	N	49	ASN
1	N	53	ASN
1	N	58	PHE
1	N	86	PHE
1	N	87	ASN
1	N	106	MET
1	N	135	LEU
1	N	184	SER
1	N	223	TYR
1	N	281	ASP
1	N	307	PHE
1	N	342	TRP
1	N	388	ARG
1	N	395	TRP
1	N	431	LEU
1	N	432	LEU
1	N	443	TRP
2	O	19	PRO
2	O	31	ASN
2	O	102	ARG
2	O	124	LEU
2	O	154	SER
2	O	160	LEU
2	O	248	ASN
2	O	296	TYR
2	O	403	ASP
3	P	21	ASP
3	P	81	ARG
3	P	91	PHE
3	P	149	ASN
3	P	182	LEU
3	P	187	PRO
3	P	199	THR
3	P	207	ASN
3	P	213	SER
3	P	234	THR
3	P	236	MET
3	P	256	ASN
3	P	259	PRO
4	Q	3	LEU
4	Q	43	MET

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Mol	Chain	Res	Type
4	Q	169	LEU
4	Q	241	LYS
5	R	6	THR
5	R	52	LYS
5	R	59	ILE
5	R	65	SER
5	R	69	LEU
5	R	80	ASP
5	R	135	LEU
6	S	13	MET
6	S	70	LEU
6	S	91	GLU
7	T	4	PHE
7	T	16	TYR
7	T	29	ILE
7	T	41	PHE
7	T	63	THR
7	T	77	TYR
8	U	26	GLN
8	U	49	HIS
10	W	11	SER
10	W	22	LEU
10	W	59	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (95) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	49	ASN
1	A	87	ASN
1	A	118	GLN
1	A	136	GLN
1	A	159	GLN
1	A	173	ASN
1	A	274	ASN
1	A	308	GLN
1	A	339	GLN
1	A	435	ASN
2	B	31	ASN
2	B	153	GLN
2	B	156	GLN
2	B	162	ASN

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Mol	Chain	Res	Type
2	B	222	GLN
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	363	GLN
2	B	376	GLN
2	B	400	GLN
3	C	17	ASN
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	105	ASN
5	E	57	GLN
5	E	86	ASN
5	E	107	ASN
5	E	164	HIS
5	E	186	GLN
6	F	79	GLN
7	G	23	GLN
7	G	44	GLN
7	G	73	ASN
7	G	79	ASN
7	G	81	GLN
8	H	75	ASN
9	I	71	ASN
1	N	10	ASN
1	N	49	ASN
1	N	85	HIS
1	N	87	ASN
1	N	118	GLN
1	N	136	GLN
1	N	159	GLN
1	N	173	ASN
1	N	274	ASN

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Mol	Chain	Res	Type
1	N	308	GLN
1	N	339	GLN
2	O	31	ASN
2	O	153	GLN
2	O	156	GLN
2	O	222	GLN
2	O	225	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	363	GLN
2	O	376	GLN
2	O	400	GLN
3	P	17	ASN
3	P	69	HIS
3	P	82	ASN
3	P	207	ASN
3	P	313	GLN
3	P	332	ASN
3	P	342	GLN
4	Q	35	GLN
4	Q	50	ASN
4	Q	105	ASN
5	R	57	GLN
5	R	86	ASN
5	R	107	ASN
5	R	164	HIS
5	R	186	GLN
6	S	79	GLN
6	S	108	ASN
7	T	12	HIS
7	T	23	GLN
7	T	44	GLN
7	T	73	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)

Of 38 ligands modelled in this entry, 12 are unknown - leaving 26 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
11	PEE	A	2008	-	20,20,50	1.70	6 (30%)	21,25,55	0.67	0
14	3H1	C	2001	-	28,29,29	2.60	13 (46%)	30,43,43	1.55	5 (16%)
14	3H1	C	2002	-	28,29,29	2.29	14 (50%)	30,43,43	1.45	7 (23%)
15	CDL	C	2003	-	49,49,99	1.19	3 (6%)	51,61,111	0.90	2 (3%)
11	PEE	C	2007	-	48,48,50	1.29	7 (14%)	49,53,55	0.90	4 (8%)
16	GOL	C	2011	-	5,5,5	1.41	0	5,5,5	0.71	0
13	HEM	C	501	3	30,50,50	2.65	9 (30%)	24,82,82	2.79	11 (45%)
13	HEM	C	502	3	30,50,50	2.77	10 (33%)	24,82,82	2.25	8 (33%)
18	BOG	D	2009	-	20,20,20	0.75	0	25,25,25	0.86	2 (8%)
17	HEC	D	501	4	24,50,50	2.85	3 (12%)	19,82,82	3.39	5 (26%)
11	PEE	E	2005	-	49,49,50	1.39	9 (18%)	50,54,55	0.95	5 (10%)
19	FES	E	501	5	0,4,4	0.00	-	0,4,4	0.00	-
15	CDL	G	2004	-	39,39,99	1.32	6 (15%)	41,51,111	1.13	4 (9%)
14	3H1	P	3001	-	28,29,29	2.67	15 (53%)	30,43,43	1.40	5 (16%)
14	3H1	P	3002	-	28,29,29	2.31	12 (42%)	30,43,43	1.50	8 (26%)
15	CDL	P	3003	-	49,49,99	1.15	2 (4%)	51,61,111	0.94	2 (3%)
11	PEE	P	3007	-	48,48,50	1.28	7 (14%)	49,53,55	0.87	4 (8%)
11	PEE	P	3008	-	4,4,50	3.76	4 (100%)	6,6,55	0.48	0
16	GOL	P	3011	-	5,5,5	1.25	0	5,5,5	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
13	HEM	P	501	3	30,50,50	3.07	12 (40%)	24,82,82	2.44	10 (41%)
13	HEM	P	502	3	30,50,50	3.10	8 (26%)	24,82,82	2.33	8 (33%)
17	HEC	Q	501	4	24,50,50	2.35	4 (16%)	19,82,82	3.17	4 (21%)
11	PEE	R	3005	-	49,49,50	1.40	9 (18%)	50,54,55	0.95	5 (10%)
18	BOG	R	3009	-	20,20,20	1.07	2 (10%)	25,25,25	1.00	2 (8%)
19	FES	R	501	5	0,4,4	0.00	-	0,4,4	0.00	-
15	CDL	T	3004	-	39,39,99	1.25	4 (10%)	41,51,111	1.16	5 (12%)

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
11	PEE	A	2008	-	-	0/24/24/54	0/0/0/0
14	3H1	C	2001	-	-	0/13/34/34	0/2/2/2
14	3H1	C	2002	-	-	0/13/34/34	0/2/2/2
15	CDL	C	2003	-	-	0/59/59/110	0/0/0/0
11	PEE	C	2007	-	-	0/52/52/54	0/0/0/0
16	GOL	C	2011	-	-	0/4/4/4	0/0/0/0
13	HEM	C	501	3	-	0/10/54/54	0/0/8/8
13	HEM	C	502	3	-	0/10/54/54	0/0/8/8
18	BOG	D	2009	-	-	0/11/31/31	0/1/1/1
17	HEC	D	501	4	-	0/6/54/54	0/0/8/8
11	PEE	E	2005	-	-	0/53/53/54	0/0/0/0
19	FES	E	501	5	-	0/0/4/4	0/1/1/1
15	CDL	G	2004	-	-	0/49/49/110	0/0/0/0
14	3H1	P	3001	-	-	0/13/34/34	0/2/2/2
14	3H1	P	3002	-	-	0/13/34/34	0/2/2/2
15	CDL	P	3003	-	-	0/59/59/110	0/0/0/0
11	PEE	P	3007	-	-	0/52/52/54	0/0/0/0
11	PEE	P	3008	-	-	0/0/0/54	0/0/0/0
16	GOL	P	3011	-	-	0/4/4/4	0/0/0/0
13	HEM	P	501	3	-	0/10/54/54	0/0/8/8
13	HEM	P	502	3	-	0/10/54/54	0/0/8/8
17	HEC	Q	501	4	-	0/6/54/54	0/0/8/8
11	PEE	R	3005	-	-	0/53/53/54	0/0/0/0
18	BOG	R	3009	-	-	0/11/31/31	0/1/1/1
19	FES	R	501	5	-	0/0/4/4	0/1/1/1
15	CDL	T	3004	-	-	0/49/49/110	0/0/0/0

All (159) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	D	501	HEC	C3B-C2B	-9.47	1.30	1.40
17	Q	501	HEC	C3B-C2B	-9.07	1.31	1.40
13	P	502	HEM	C3B-C4B	-9.05	1.43	1.51
17	D	501	HEC	C3C-C2C	-8.91	1.31	1.40
13	C	501	HEM	C3B-CAB	-7.68	1.36	1.51
13	P	501	HEM	C3B-CAB	-7.60	1.37	1.51
13	C	502	HEM	C3B-CAB	-7.47	1.37	1.51
13	P	502	HEM	C3B-CAB	-7.27	1.37	1.51
13	P	501	HEM	C2D-C3D	-6.59	1.34	1.54
13	P	501	HEM	C3C-CAC	-6.44	1.39	1.51
13	C	501	HEM	C3C-CAC	-6.15	1.39	1.51
13	C	502	HEM	C2C-C1C	-6.12	1.40	1.52
13	P	502	HEM	C2D-C3D	-6.04	1.36	1.54
13	C	502	HEM	C3C-CAC	-6.00	1.40	1.51
13	C	501	HEM	C2D-C3D	-5.98	1.36	1.54
13	C	502	HEM	C2D-C3D	-5.95	1.36	1.54
13	P	502	HEM	C3C-CAC	-5.70	1.40	1.51
13	P	501	HEM	C3B-C4B	-5.63	1.46	1.51
13	P	501	HEM	C3D-C4D	-5.21	1.44	1.51
17	Q	501	HEC	C3C-C2C	-4.92	1.35	1.40
13	P	502	HEM	C2C-C1C	-4.87	1.43	1.52
14	P	3002	3H1	C17-C15	-4.69	1.35	1.45
14	C	2001	3H1	C17-C15	-4.66	1.35	1.45
14	C	2002	3H1	C17-C15	-4.39	1.36	1.45
14	P	3001	3H1	C17-C15	-4.27	1.36	1.45
13	P	502	HEM	C3D-C4D	-3.50	1.47	1.51
13	C	501	HEM	C3D-C4D	-3.34	1.47	1.51
13	C	502	HEM	C3B-C4B	-3.06	1.49	1.51
11	P	3007	PEE	C19-C18	-2.93	1.34	1.51
11	E	2005	PEE	C19-C18	-2.92	1.34	1.51
11	C	2007	PEE	C19-C18	-2.89	1.34	1.51
11	R	3005	PEE	C19-C18	-2.89	1.34	1.51
13	P	501	HEM	C2B-C1B	-2.88	1.42	1.51
11	P	3007	PEE	C22-C21	-2.87	1.34	1.51
11	E	2005	PEE	C22-C21	-2.72	1.35	1.51
11	C	2007	PEE	C22-C21	-2.68	1.36	1.51
11	R	3005	PEE	C22-C21	-2.68	1.36	1.51
13	C	501	HEM	C2C-C1C	-2.64	1.47	1.52
15	G	2004	CDL	OA8-CA6	-2.39	1.39	1.45
13	C	502	HEM	C3D-C4D	-2.38	1.48	1.51
15	T	3004	CDL	OA8-CA6	-2.36	1.39	1.45
13	C	502	HEM	C2A-C3A	-2.32	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	C	502	HEM	C2D-C1D	-2.27	1.44	1.51
13	P	501	HEM	C2D-C1D	-2.15	1.44	1.51
15	C	2003	CDL	OA2-CA2	-2.08	1.36	1.44
13	C	501	HEM	FE-NB	-2.05	1.86	1.97
15	P	3003	CDL	OA2-CA2	-2.03	1.36	1.44
17	Q	501	HEC	C4D-CHA	-2.00	1.34	1.39
11	P	3007	PEE	C3-C2	2.00	1.56	1.50
11	P	3007	PEE	C1-C2	2.00	1.56	1.50
14	P	3002	3H1	C02-C01	2.02	1.43	1.40
11	C	2007	PEE	P-O2P	2.03	1.63	1.54
14	C	2002	3H1	C16-C15	2.04	1.55	1.50
14	P	3001	3H1	C08-C03	2.04	1.55	1.51
15	C	2003	CDL	CA3-CA4	2.05	1.56	1.50
11	E	2005	PEE	C11-C10	2.06	1.56	1.50
11	R	3005	PEE	C1-C2	2.07	1.56	1.50
11	P	3008	PEE	P-O2P	2.07	1.62	1.54
17	Q	501	HEC	C3C-C4C	2.08	1.47	1.42
18	R	3009	BOG	C1-C2	2.08	1.58	1.52
11	A	2008	PEE	C3-C2	2.10	1.56	1.50
14	C	2002	3H1	C02-C01	2.10	1.43	1.40
15	T	3004	CDL	OB8-CB7	2.12	1.39	1.33
11	A	2008	PEE	C11-C10	2.15	1.57	1.50
15	G	2004	CDL	CB3-CB4	2.15	1.56	1.50
14	P	3002	3H1	C13-C06	2.16	1.54	1.51
14	P	3001	3H1	C27-C24	2.16	1.57	1.53
14	C	2002	3H1	C27-C24	2.18	1.57	1.53
14	C	2002	3H1	C08-C03	2.19	1.56	1.51
15	G	2004	CDL	OB8-CB7	2.20	1.39	1.33
17	D	501	HEC	C3C-C4C	2.21	1.47	1.42
15	T	3004	CDL	O1-C1	2.21	1.50	1.43
11	C	2007	PEE	C1-C2	2.21	1.57	1.50
11	E	2005	PEE	C31-C30	2.26	1.57	1.50
14	C	2002	3H1	C22-C23	2.27	1.54	1.50
11	C	2007	PEE	P-O1P	2.28	1.59	1.51
15	G	2004	CDL	O1-C1	2.30	1.50	1.43
11	R	3005	PEE	C31-C30	2.32	1.57	1.50
14	P	3002	3H1	C04-CL12	2.33	1.77	1.72
13	P	501	HEM	CHC-C1C	2.33	1.41	1.36
14	C	2001	3H1	C08-C03	2.34	1.56	1.51
11	A	2008	PEE	O3-C30	2.36	1.40	1.33
11	E	2005	PEE	C1-C2	2.38	1.57	1.50
14	C	2002	3H1	C01-C06	2.39	1.43	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	E	2005	PEE	C3-C2	2.40	1.57	1.50
14	P	3001	3H1	C02-C03	2.42	1.44	1.41
13	C	501	HEM	C4C-NC	2.42	1.39	1.36
15	P	3003	CDL	CA3-CA4	2.43	1.57	1.50
15	G	2004	CDL	OA6-CA5	2.45	1.41	1.34
15	C	2003	CDL	OB8-CB7	2.45	1.40	1.33
14	C	2001	3H1	C02-C01	2.45	1.43	1.40
11	R	3005	PEE	C11-C10	2.48	1.58	1.50
14	C	2001	3H1	C24-C23	2.49	1.55	1.52
11	P	3007	PEE	P-O1P	2.52	1.60	1.51
14	C	2001	3H1	C28-C19	2.53	1.58	1.54
11	R	3005	PEE	C3-C2	2.58	1.58	1.50
14	C	2002	3H1	C19-C18	2.59	1.55	1.51
14	P	3002	3H1	C02-C07	2.61	1.52	1.46
14	C	2001	3H1	C02-C03	2.63	1.45	1.41
11	A	2008	PEE	C1-C2	2.66	1.58	1.50
14	C	2002	3H1	C19-C20	2.67	1.62	1.57
13	C	502	HEM	CBB-CAB	2.69	1.44	1.29
15	G	2004	CDL	CA3-CA4	2.71	1.58	1.50
14	C	2001	3H1	C01-C06	2.76	1.44	1.40
11	A	2008	PEE	P-O1P	2.77	1.61	1.51
11	P	3008	PEE	P-O3P	2.78	1.64	1.54
14	P	3002	3H1	C19-C18	2.81	1.55	1.51
11	P	3008	PEE	P-O4P	2.81	1.64	1.54
11	E	2005	PEE	P-O1P	2.81	1.61	1.51
14	P	3001	3H1	C04-C03	2.82	1.43	1.39
14	P	3002	3H1	C22-C23	2.82	1.55	1.50
14	P	3001	3H1	C02-C01	2.83	1.44	1.40
14	P	3001	3H1	C22-C23	2.86	1.55	1.50
14	C	2002	3H1	C04-CL12	2.86	1.78	1.72
13	P	501	HEM	C1C-NC	2.93	1.39	1.36
14	P	3001	3H1	C19-C20	2.93	1.62	1.57
15	T	3004	CDL	CA3-CA4	2.96	1.59	1.50
14	C	2002	3H1	C02-C03	3.00	1.45	1.41
11	E	2005	PEE	O2-C10	3.01	1.43	1.34
18	R	3009	BOG	C4-C5	3.04	1.59	1.53
14	C	2001	3H1	C05-C06	3.04	1.44	1.40
11	P	3007	PEE	O2-C10	3.05	1.43	1.34
14	P	3001	3H1	C21-C20	3.07	1.58	1.53
14	P	3002	3H1	C28-C19	3.14	1.58	1.54
14	P	3001	3H1	C05-C06	3.16	1.44	1.40
11	P	3007	PEE	O3-C30	3.17	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	P	3001	3H1	C28-C19	3.17	1.59	1.54
11	C	2007	PEE	O3-C30	3.18	1.42	1.33
11	R	3005	PEE	P-O1P	3.19	1.62	1.51
11	R	3005	PEE	O3-C30	3.21	1.43	1.33
11	R	3005	PEE	O2-C10	3.23	1.44	1.34
13	P	501	HEM	C4C-NC	3.24	1.40	1.36
14	P	3002	3H1	C02-C03	3.26	1.46	1.41
14	P	3001	3H1	C04-CL12	3.30	1.79	1.72
14	C	2002	3H1	C28-C19	3.30	1.59	1.54
11	A	2008	PEE	O2-C10	3.34	1.44	1.34
11	C	2007	PEE	O2-C10	3.36	1.44	1.34
11	E	2005	PEE	O3-C30	3.37	1.43	1.33
13	C	501	HEM	CBB-CAB	3.38	1.48	1.29
14	P	3002	3H1	C04-C03	3.39	1.44	1.39
14	C	2001	3H1	C21-C20	3.43	1.58	1.53
13	P	501	HEM	CBC-CAC	3.45	1.49	1.29
14	P	3002	3H1	C19-C20	3.50	1.63	1.57
13	P	502	HEM	CBB-CAB	3.51	1.49	1.29
14	P	3001	3H1	C24-C23	3.75	1.57	1.52
14	C	2001	3H1	C04-CL12	3.97	1.81	1.72
13	C	501	HEM	CBC-CAC	4.05	1.52	1.29
13	P	502	HEM	CBC-CAC	4.08	1.52	1.29
13	P	501	HEM	CBB-CAB	4.22	1.53	1.29
14	C	2002	3H1	C21-C20	4.23	1.60	1.53
14	P	3001	3H1	C19-C18	4.23	1.57	1.51
13	C	502	HEM	CBC-CAC	4.27	1.54	1.29
14	C	2001	3H1	C19-C18	4.30	1.58	1.51
14	P	3002	3H1	C21-C20	4.31	1.60	1.53
14	C	2002	3H1	C04-C03	4.44	1.45	1.39
14	C	2001	3H1	C04-C03	4.55	1.45	1.39
14	C	2001	3H1	C13-C06	4.95	1.57	1.51
14	P	3001	3H1	C13-C06	5.81	1.58	1.51
11	P	3008	PEE	P-O1P	6.05	1.62	1.50

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	Q	501	HEC	CBC-CAC-C3C	-8.64	108.15	127.35
17	D	501	HEC	CBB-CAB-C3B	-8.05	109.45	127.35
17	D	501	HEC	CBC-CAC-C3C	-7.90	109.79	127.35
17	Q	501	HEC	CBB-CAB-C3B	-7.53	110.63	127.35
13	C	501	HEM	C3B-CAB-CBB	-6.73	114.13	124.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	C	501	HEM	CBA-CAA-C2A	-4.98	103.61	112.53
13	P	501	HEM	C3B-CAB-CBB	-4.30	117.86	124.46
14	C	2001	3H1	C05-C04-C03	-4.03	119.02	122.56
13	P	501	HEM	CBA-CAA-C2A	-3.74	105.83	112.53
17	D	501	HEC	CAA-C2A-C3A	-3.69	118.47	129.00
13	P	502	HEM	CBD-CAD-C3D	-3.54	103.25	113.55
15	T	3004	CDL	CB4-OB6-CB5	-3.11	110.43	117.89
17	Q	501	HEC	CAA-C2A-C3A	-3.06	120.26	129.00
13	C	502	HEM	C3B-CAB-CBB	-2.99	119.87	124.46
14	C	2002	3H1	C05-C04-C03	-2.97	119.94	122.56
14	P	3001	3H1	C05-C04-C03	-2.97	119.94	122.56
13	C	502	HEM	CBD-CAD-C3D	-2.94	105.00	113.55
14	C	2001	3H1	C27-C24-C23	-2.94	106.30	111.33
15	C	2003	CDL	CB4-OB6-CB5	-2.92	110.89	117.89
14	P	3001	3H1	C25-C20-C21	-2.81	105.92	110.44
15	G	2004	CDL	CB6-CB4-CB3	-2.71	105.73	112.07
14	P	3002	3H1	C25-C20-C21	-2.69	106.11	110.44
14	P	3002	3H1	C05-C04-C03	-2.68	120.21	122.56
15	P	3003	CDL	CB4-OB6-CB5	-2.68	111.47	117.89
14	P	3001	3H1	C27-C24-C23	-2.49	107.06	111.33
14	C	2002	3H1	C25-C20-C21	-2.49	106.43	110.44
14	P	3002	3H1	C27-C24-C23	-2.42	107.19	111.33
15	T	3004	CDL	CA6-OA8-CA7	-2.33	111.25	117.14
14	C	2002	3H1	C27-C24-C23	-2.32	107.35	111.33
14	C	2002	3H1	C13-C06-C05	-2.31	118.07	121.01
15	G	2004	CDL	CB4-OB6-CB5	-2.30	112.36	117.89
15	G	2004	CDL	CA6-CA4-CA3	-2.28	106.74	112.07
15	G	2004	CDL	CA6-OA8-CA7	-2.27	111.39	117.14
15	P	3003	CDL	CA6-CA4-CA3	-2.27	106.75	112.07
15	T	3004	CDL	CB6-CB4-CB3	-2.26	106.78	112.07
15	T	3004	CDL	CA6-CA4-CA3	-2.20	106.94	112.07
14	C	2001	3H1	C25-C20-C21	-2.16	106.95	110.44
13	C	501	HEM	CMA-C3A-C4A	-2.12	124.86	128.36
15	C	2003	CDL	CA6-CA4-CA3	-2.08	107.20	112.07
14	P	3002	3H1	C13-C06-C05	-2.04	118.41	121.01
14	P	3002	3H1	C08-C03-C04	-2.01	118.33	121.42
15	T	3004	CDL	OA6-CA4-CA3	2.04	115.55	108.36
13	P	501	HEM	C2C-C1C-CHC	2.05	126.80	123.68
14	C	2002	3H1	C16-C15-C17	2.12	121.63	118.10
18	D	2009	BOG	O1-C1-C2	2.13	110.72	108.04
13	C	501	HEM	CMA-C3A-C2A	2.21	129.85	125.24
14	P	3002	3H1	C22-C21-C20	2.23	117.25	112.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	C	502	HEM	CBA-CAA-C2A	2.25	116.56	112.53
14	C	2002	3H1	C22-C21-C20	2.28	117.34	112.46
11	R	3005	PEE	O3-C3-C2	2.28	114.82	108.69
11	P	3007	PEE	C23-C22-C21	2.32	126.53	114.53
14	P	3002	3H1	C16-C15-C17	2.33	121.98	118.10
18	R	3009	BOG	O1-C1-C2	2.34	110.99	108.04
11	P	3007	PEE	C22-C21-C20	2.36	126.71	114.53
11	E	2005	PEE	C19-C18-C17	2.37	126.76	114.53
14	P	3001	3H1	C03-C04-CL12	2.40	122.29	118.66
11	R	3005	PEE	C19-C18-C17	2.40	126.93	114.53
11	C	2007	PEE	C22-C21-C20	2.41	126.95	114.53
11	E	2005	PEE	O3-C3-C2	2.42	115.20	108.69
13	C	501	HEM	CBD-CAD-C3D	2.45	120.68	113.55
11	C	2007	PEE	C23-C22-C21	2.46	127.23	114.53
11	E	2005	PEE	C23-C22-C21	2.46	127.25	114.53
13	C	502	HEM	CMD-C2D-C3D	2.47	125.28	114.35
11	R	3005	PEE	C23-C22-C21	2.50	127.42	114.53
13	P	501	HEM	C3B-C4B-CHC	2.51	126.70	123.16
11	R	3005	PEE	C22-C21-C20	2.51	127.52	114.53
11	E	2005	PEE	C22-C21-C20	2.55	127.70	114.53
13	P	502	HEM	C2D-C3D-C4D	2.60	105.90	101.50
14	P	3002	3H1	C03-C04-CL12	2.60	122.60	118.66
18	D	2009	BOG	C1'-O1-C1	2.61	118.50	113.94
11	P	3007	PEE	C19-C18-C17	2.62	128.05	114.53
11	P	3007	PEE	C20-C19-C18	2.65	128.22	114.53
11	C	2007	PEE	C19-C18-C17	2.66	128.29	114.53
11	C	2007	PEE	C20-C19-C18	2.67	128.34	114.53
14	P	3001	3H1	C16-C15-C17	2.70	122.59	118.10
11	E	2005	PEE	C20-C19-C18	2.72	128.57	114.53
13	P	502	HEM	CMD-C2D-C3D	2.72	126.37	114.35
13	C	501	HEM	CMD-C2D-C3D	2.73	126.43	114.35
14	C	2001	3H1	C16-C15-C17	2.73	122.65	118.10
13	P	501	HEM	CMD-C2D-C3D	2.77	126.59	114.35
11	R	3005	PEE	C20-C19-C18	2.77	128.84	114.53
14	C	2002	3H1	C03-C04-CL12	2.80	122.90	118.66
13	P	502	HEM	CBA-CAA-C2A	2.98	117.87	112.53
13	P	501	HEM	C2D-C3D-C4D	3.02	106.61	101.50
13	C	501	HEM	C2D-C3D-C4D	3.08	106.72	101.50
18	R	3009	BOG	C1'-O1-C1	3.18	119.51	113.94
14	C	2001	3H1	C03-C04-CL12	3.65	124.18	118.66
13	C	501	HEM	CMC-C2C-C3C	3.66	125.68	116.53
13	P	501	HEM	CAD-C3D-C4D	3.68	125.46	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	C	501	HEM	CAD-C3D-C4D	3.85	126.05	112.47
13	P	502	HEM	CAD-C3D-C2D	3.96	124.59	113.22
17	D	501	HEC	CAD-C3D-C4D	3.96	131.31	127.01
13	P	501	HEM	CMB-C2B-C3B	4.06	126.67	116.53
13	C	502	HEM	CAD-C3D-C2D	4.12	125.06	113.22
13	C	502	HEM	CMC-C2C-C3C	4.16	126.91	116.53
13	P	502	HEM	CAD-C3D-C4D	4.52	128.41	112.47
13	C	501	HEM	CAD-C3D-C2D	4.60	126.43	113.22
13	C	502	HEM	CMB-C2B-C3B	4.60	128.00	116.53
13	P	502	HEM	CMC-C2C-C3C	4.62	128.07	116.53
13	P	501	HEM	CMC-C2C-C3C	4.68	128.21	116.53
13	P	501	HEM	CAD-C3D-C2D	4.86	127.20	113.22
13	C	502	HEM	CAD-C3D-C4D	4.94	129.88	112.47
13	C	501	HEM	CMB-C2B-C3B	4.94	128.87	116.53
13	P	502	HEM	CMB-C2B-C3B	5.11	129.29	116.53
17	Q	501	HEC	CAA-C2A-C1A	6.00	133.52	127.01
17	D	501	HEC	CAA-C2A-C1A	6.97	134.58	127.01

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

20 monomers are involved in 52 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	C	2001	3H1	2	0
14	C	2002	3H1	1	0
15	C	2003	CDL	2	0
13	C	501	HEM	7	0
13	C	502	HEM	5	0
18	D	2009	BOG	1	0
17	D	501	HEC	3	0
19	E	501	FES	1	0
15	G	2004	CDL	1	0
14	P	3001	3H1	4	0
14	P	3002	3H1	5	0
15	P	3003	CDL	1	0
11	P	3007	PEE	3	0
13	P	501	HEM	5	0
13	P	502	HEM	2	0
17	Q	501	HEC	3	0
11	R	3005	PEE	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	R	3009	BOG	1	0
19	R	501	FES	1	0
15	T	3004	CDL	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	443/446 (99%)	0.06	14 (3%) 51 38	56, 105, 138, 156	0
1	N	442/446 (99%)	0.08	15 (3%) 49 35	66, 108, 138, 151	0
2	B	421/441 (95%)	0.12	19 (4%) 37 25	85, 124, 160, 177	0
2	O	422/441 (95%)	0.17	17 (4%) 42 29	68, 111, 142, 167	0
3	C	380/380 (100%)	-0.26	7 (1%) 71 60	39, 61, 113, 164	0
3	P	379/380 (99%)	-0.02	8 (2%) 67 54	59, 104, 140, 164	0
4	D	241/241 (100%)	-0.31	3 (1%) 81 71	53, 68, 111, 136	0
4	Q	241/241 (100%)	-0.04	4 (1%) 73 62	84, 117, 150, 163	0
5	E	196/196 (100%)	0.83	34 (17%) 2 1	63, 142, 190, 194	0
5	R	196/196 (100%)	0.29	17 (8%) 13 8	64, 107, 152, 165	0
6	F	101/110 (91%)	-0.41	0 100 100	52, 68, 86, 121	0
6	S	101/110 (91%)	0.37	4 (3%) 42 29	96, 122, 162, 177	0
7	G	81/81 (100%)	-0.03	1 (1%) 81 71	53, 74, 134, 148	0
7	T	79/81 (97%)	0.71	12 (15%) 3 2	89, 132, 184, 194	0
8	H	70/77 (90%)	-0.29	1 (1%) 78 67	56, 95, 116, 154	0
8	U	67/77 (87%)	0.65	6 (8%) 12 7	143, 165, 185, 187	0
9	I	31/47 (65%)	1.33	8 (25%) 1 1	128, 157, 170, 174	0
9	V	31/47 (65%)	1.59	10 (32%) 1 1	109, 147, 196, 198	0
10	J	61/61 (100%)	-0.15	1 (1%) 74 64	73, 93, 137, 168	0
10	W	59/61 (96%)	0.53	7 (11%) 6 4	91, 109, 133, 159	0
All	All	4042/4160 (97%)	0.10	188 (4%) 35 24	39, 106, 160, 198	0

All (188) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	T	1	GLY	10.1
5	E	111	GLU	8.0
5	E	109	GLU	7.9
9	I	48	PRO	7.6
5	E	110	ALA	7.1
10	W	62	SER	6.7
9	V	48	PRO	6.6
3	P	7	LYS	6.4
5	E	112	VAL	6.4
7	T	78	GLU	6.1
1	A	2	ALA	5.3
9	I	47	ARG	5.1
7	T	74	PRO	5.1
2	B	402	ILE	5.0
8	U	12	GLU	4.9
1	A	35	CYS	4.8
7	T	2	ILE	4.8
3	P	8	SER	4.8
8	U	50	THR	4.7
5	E	172	ARG	4.7
5	R	120	PRO	4.7
8	U	13	LEU	4.6
5	E	132	TRP	4.5
1	N	177	LEU	4.5
5	E	114	VAL	4.5
1	N	174	ILE	4.4
10	W	60	GLU	4.4
3	C	1	MET	4.3
9	V	54	SER	4.2
5	R	121	GLN	4.2
5	E	173	LYS	4.1
2	B	393	THR	4.1
2	B	216	LEU	4.1
9	V	47	ARG	4.1
9	V	49	LEU	4.0
3	C	6	ARG	4.0
5	R	114	VAL	3.9
5	E	122	HIS	3.9
2	O	268	GLU	3.9
7	T	73	ASN	3.9
3	C	5	ILE	3.9
2	B	398	VAL	3.8
1	A	69	LYS	3.8

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Mol	Chain	Res	Type	RSRZ
2	B	439	LEU	3.8
3	C	8	SER	3.8
5	E	77	LYS	3.8
5	R	117	LEU	3.7
2	B	396	SER	3.7
5	E	121	GLN	3.7
4	D	241	LYS	3.6
5	E	137	GLY	3.6
9	V	62	ARG	3.5
3	P	6	ARG	3.5
1	N	117	VAL	3.5
5	E	78	LEU	3.5
1	N	57	TYR	3.4
7	T	77	TYR	3.4
9	I	76	VAL	3.4
4	Q	145	GLU	3.4
1	N	386	TYR	3.4
2	B	395	PRO	3.4
1	A	102	LEU	3.4
7	T	71	ARG	3.4
2	B	349	GLN	3.3
5	E	134	ILE	3.3
9	I	63	ASP	3.3
3	P	4	ASN	3.3
1	N	66	GLY	3.2
1	N	131	ARG	3.2
6	S	15	ARG	3.1
5	E	125	ASP	3.1
6	S	89	TYR	3.1
1	A	8	LEU	3.1
9	V	50	LEU	3.1
3	C	7	LYS	3.1
7	T	3	HIS	3.1
5	E	188	VAL	3.1
4	Q	146	GLY	3.1
7	T	24	ARG	3.1
5	E	136	VAL	3.0
5	E	174	GLY	3.0
5	R	113	ASP	3.0
10	J	64	GLU	3.0
8	U	54	CYS	3.0
9	V	77	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
9	V	63	ASP	3.0
7	T	72	LYS	3.0
5	E	187	PHE	2.9
2	O	410	VAL	2.9
3	P	3	PRO	2.9
3	P	29	SER	2.9
5	R	122	HIS	2.9
3	P	157	ILE	2.9
5	R	118	ARG	2.9
5	R	119	ASP	2.9
3	C	4	ASN	2.8
5	E	165	TYR	2.8
2	B	36	ALA	2.8
7	T	75	ALA	2.8
1	A	216	PHE	2.8
1	A	174	ILE	2.7
1	A	177	LEU	2.7
1	N	75	PHE	2.7
2	O	252	LEU	2.7
5	E	113	ASP	2.7
2	O	352	VAL	2.7
6	S	12	LEU	2.7
7	T	53	LEU	2.7
2	O	386	ALA	2.7
2	O	23	ASP	2.6
2	B	206	LEU	2.6
2	O	413	ALA	2.6
8	U	44	VAL	2.6
4	D	240	PRO	2.6
5	E	163	SER	2.6
5	E	76	ILE	2.6
5	E	167	ALA	2.6
9	V	61	ARG	2.6
1	N	182	LEU	2.6
2	B	365	LYS	2.6
5	E	75	GLU	2.6
6	S	110	LYS	2.6
9	I	61	ARG	2.6
1	N	195	MET	2.6
2	O	283	PRO	2.6
1	N	216	PHE	2.5
3	P	2	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	345	LYS	2.5
5	E	169	GLY	2.5
10	W	61	ALA	2.5
4	Q	17	PRO	2.5
5	E	1	VAL	2.5
5	R	195	VAL	2.5
1	A	208	LEU	2.5
5	E	127	VAL	2.5
9	I	77	ARG	2.5
2	B	401	LYS	2.5
5	E	70	ALA	2.4
8	U	24	CYS	2.4
2	O	36	ALA	2.4
4	Q	167	GLU	2.4
10	W	56	LYS	2.4
5	E	191	ASP	2.4
2	B	185	LYS	2.4
2	O	347	ALA	2.3
10	W	33	ARG	2.3
5	R	74	ILE	2.3
5	R	112	VAL	2.3
1	A	4	TYR	2.3
2	O	416	LYS	2.3
2	O	274	VAL	2.3
2	O	267	ALA	2.3
2	B	350	GLY	2.3
5	R	109	GLU	2.3
1	N	390	ILE	2.2
1	A	5	ALA	2.2
8	H	71	HIS	2.2
5	E	162	GLY	2.2
1	N	379	ILE	2.2
5	R	194	VAL	2.2
2	B	397	VAL	2.2
2	O	414	ALA	2.2
1	A	142	ASP	2.2
5	R	170	ARG	2.2
5	E	79	SER	2.2
2	O	344	LEU	2.1
2	O	409	ASP	2.1
10	W	53	LYS	2.1
1	A	34	THR	2.1

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Mol	Chain	Res	Type	RSRZ
3	C	59	ASP	2.1
10	W	52	TRP	2.1
5	E	90	LYS	2.1
4	D	1	GLY	2.1
2	B	352	VAL	2.1
9	V	53	GLU	2.1
7	G	38	TRP	2.1
5	E	124	LEU	2.1
2	B	368	TYR	2.1
2	O	353	THR	2.0
1	N	113	LEU	2.0
9	I	62	ARG	2.0
1	N	389	ARG	2.0
5	R	115	SER	2.0
5	R	172	ARG	2.0
2	B	211	VAL	2.0
9	I	69	SER	2.0
1	A	122	LEU	2.0
5	R	192	LEU	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
12	UNL	R	2103	1/-	0.78	0.79	40.21	53,53,53,53	0
16	GOL	C	2011	6/6	0.86	0.46	9.30	84,87,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
12	UNL	A	3016	1/-	0.86	0.54	8.55	69,69,69,69	0
11	PEE	R	3005	50/51	0.67	0.54	4.85	102,123,129,130	0
11	PEE	E	2005	50/51	0.81	0.42	4.28	95,113,124,126	0
12	UNL	P	3103	1/-	0.63	0.55	4.25	76,76,76,76	0
18	BOG	D	2009	20/20	0.93	0.23	3.53	75,88,91,92	0
16	GOL	P	3011	6/6	0.88	0.45	3.06	108,110,111,113	0
15	CDL	P	3003	50/100	0.71	0.42	2.33	150,158,162,162	0
11	PEE	C	2007	49/51	0.93	0.26	2.07	55,72,95,97	0
14	3H1	P	3002	28/28	0.79	0.34	1.82	101,108,114,114	0
11	PEE	P	3007	49/51	0.88	0.36	1.54	107,121,139,140	0
14	3H1	C	2002	28/28	0.90	0.26	1.18	66,76,89,89	0
15	CDL	C	2003	50/100	0.88	0.27	0.98	82,93,106,107	0
14	3H1	P	3001	28/28	0.89	0.29	0.87	101,106,112,112	0
15	CDL	T	3004	40/100	0.85	0.33	0.86	117,124,129,131	0
18	BOG	R	3009	20/20	0.89	0.23	0.76	101,121,124,124	0
15	CDL	G	2004	40/100	0.93	0.24	0.70	65,79,101,103	0
13	HEM	C	501	43/43	0.98	0.22	0.38	47,53,58,62	0
13	HEM	P	501	43/43	0.97	0.23	0.27	72,78,85,88	0
13	HEM	C	502	43/43	0.98	0.21	0.20	37,42,47,56	0
14	3H1	C	2001	28/28	0.93	0.21	0.20	47,56,60,61	0
17	HEC	Q	501	43/43	0.95	0.22	-0.16	95,99,103,105	0
13	HEM	P	502	43/43	0.98	0.20	-0.18	79,81,93,100	0
17	HEC	D	501	43/43	0.98	0.17	-0.28	38,48,57,60	0
19	FES	R	501	4/4	0.99	0.14	-0.66	69,69,69,69	0
19	FES	E	501	4/4	0.97	0.12	-1.47	118,119,120,120	0
12	UNL	C	3106	1/-	0.78	0.72	-	44,44,44,44	0
12	UNL	P	2015	1/-	0.83	0.23	-	48,48,48,48	0
11	PEE	P	3008	5/51	0.83	0.54	-	149,149,150,151	0
12	UNL	P	3010	1/-	0.68	0.94	-	60,60,60,60	0
12	UNL	C	3015	1/-	0.73	0.45	-	53,53,53,53	0
12	UNL	C	2010	1/-	0.93	0.50	-	30,30,30,30	0
12	UNL	P	2106	1/-	0.49	1.35	-	63,63,63,63	0
12	UNL	E	2105	1/-	0.50	0.45	-	82,82,82,82	0
12	UNL	P	3104	1/-	0.50	0.93	-	83,83,83,83	0
12	UNL	C	2104	1/-	0.38	0.74	-	85,85,85,85	0
11	PEE	A	2008	21/51	0.72	0.37	-	149,161,164,166	0

6.5 Other polymers (i)

There are no such residues in this entry.