



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:06 AM GMT

PDB ID : 3H1H  
Title : Cytochrome bc1 complex from chicken  
Authors : Zhang, Z.; Huang, L.; Shulmeister, V.M.; Chi, Y.I.; Kim, K.K.; Hung, L.W.;  
Crofts, A.R.; Berry, E.A.; Kim, S.H.  
Deposited on : 2009-04-12  
Resolution : 3.16 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (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

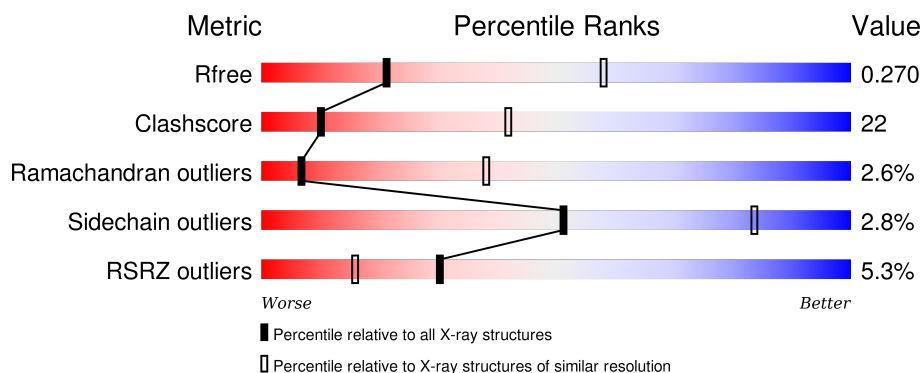
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.16 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	1112 (3.20-3.12)
Clashscore	102246	1249 (3.20-3.12)
Ramachandran outliers	100387	1222 (3.20-3.12)
Sidechain outliers	100360	1221 (3.20-3.12)
RSRZ outliers	91569	1117 (3.20-3.12)

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

Mol	Chain	Length	Quality of chain
1	A	446	<div> <div>61%</div> <div>35%</div> <div>• •</div> </div>
1	N	446	<div> <div>59%</div> <div>37%</div> <div>• •</div> </div>
2	B	441	<div> <div>3%</div> <div>49%</div> <div>42%</div> <div>• 5%</div> </div>
2	O	441	<div> <div>2%</div> <div>49%</div> <div>41%</div> <div>5% •</div> </div>
3	C	380	<div> <div>68%</div> <div>31%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
3	P	380	
4	D	241	
4	Q	241	
5	E	196	
5	R	196	
6	F	110	
6	S	110	
7	G	81	
7	T	81	
8	H	77	
8	U	77	
9	I	47	
9	V	47	
10	J	61	
10	W	61	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	UNL	A	3284	-	-	-	X
11	UNL	C	3288	-	-	-	X
13	UQ	C	2002	-	-	-	X
13	UQ	P	3002	-	-	-	X
14	CDL	D	2003	-	-	-	X
14	CDL	Q	3003	-	-	-	X
15	PEE	C	2007	-	-	-	X
15	PEE	C	2008	-	-	-	X
15	PEE	E	2005	-	-	-	X
15	PEE	N	3008	-	X	-	-
15	PEE	P	3007	-	-	-	X
15	PEE	R	3005	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	GOL	C	2011	-	-	-	X
16	GOL	P	3011	-	-	-	X
18	BOG	P	2010	-	-	-	X
19	FES	E	501	-	-	X	-
19	FES	R	501	-	-	X	-

## 2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 32608 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 UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN I, MITOCHONDRIAL.

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

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

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
			3017	2022	478	505	12			
3	P	379	Total	C	N	O	S	0	0	0
			3012	2019	477	504	12			

- Molecule 4 is a protein called CYTOCHROME C1, HEME PROTEIN, MITOCHONDRIAL.

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

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

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

- Molecule 6 is a protein called UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 14 KDA PROTEIN.

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

- Molecule 7 is a protein called UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX UBIQUINONE-BINDING PROTEIN QP-C.

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

- Molecule 8 is a protein called UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 11 KDA PROTEIN.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	46	Total	C	N	O	S	0	0	0
			287	171	58	56	2			
9	V	44	Total	C	N	O	S	0	0	1
			278	167	56	53	2			

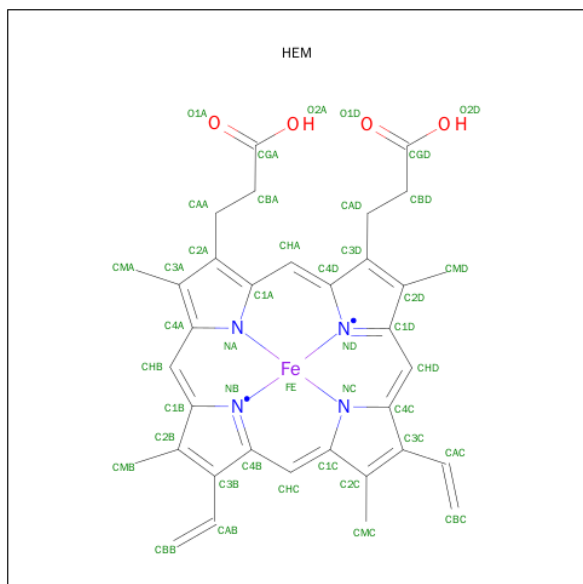
- Molecule 10 is a protein called UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 7.2 KDA PROTEIN.

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	P	1	Total	O	0	0
			1	1		
11	A	3	Total	O	0	0
			3	3		
11	C	2	Total	O	0	0
			2	2		
11	N	3	Total	O	0	0
			3	3		

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



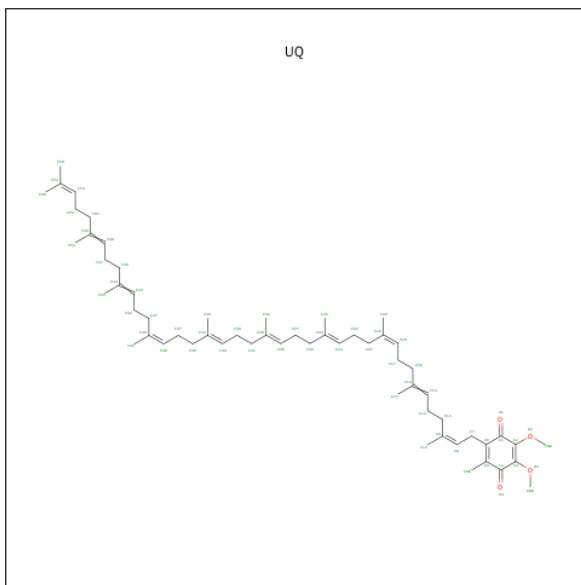
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	0
12	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	0
12	P	1	Total	C	Fe	N	O	0
			43	34	1	4	4	0

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

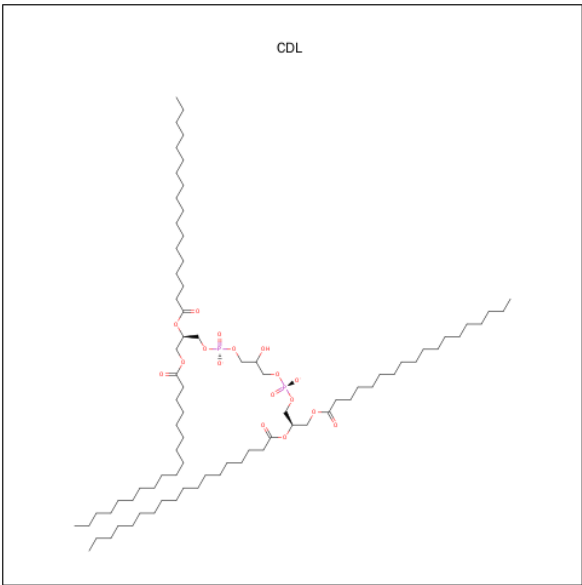
- Molecule 13 is COENZYME Q10, (2Z,6E,10Z,14E,18E,22E,26Z)-ISOMER (three-letter code: UQ) (formula: C<sub>59</sub>H<sub>90</sub>O<sub>4</sub>).



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

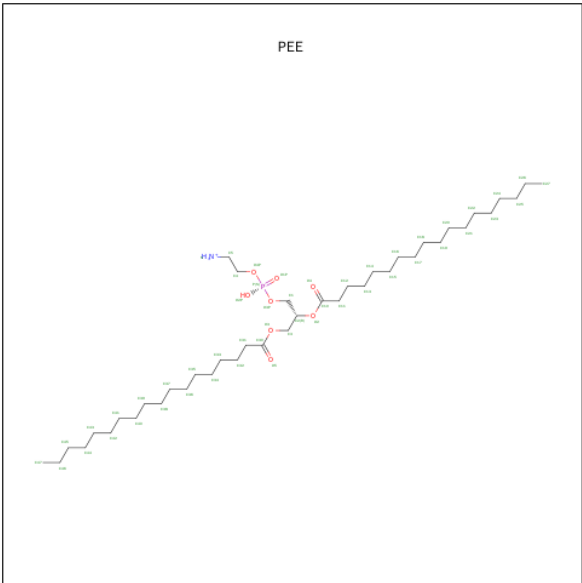
- Molecule 14 is CARDIOLIPIN (three-letter code: CDL) (formula: C<sub>81</sub>H<sub>156</sub>O<sub>17</sub>P<sub>2</sub>).





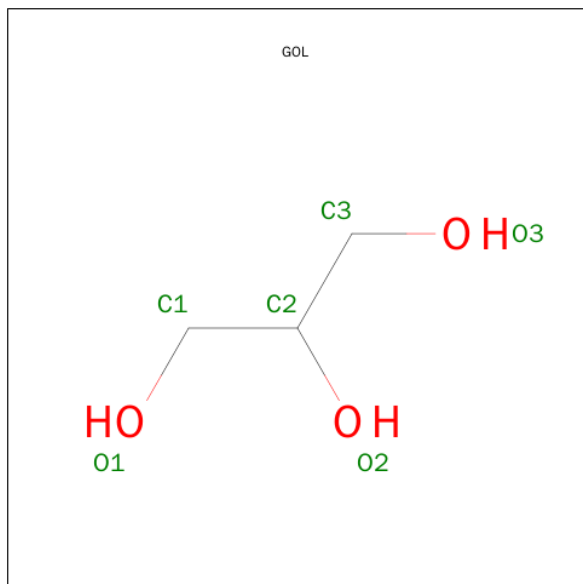
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	C	1	Total	C	O	P	0	0
			40	21	17	2		
14	D	1	Total	C	O	P	0	0
			42	23	17	2		
14	P	1	Total	C	O	P	0	0
			40	21	17	2		
14	Q	1	Total	C	O	P	0	0
			42	23	17	2		

- Molecule 15 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PEE) (formula:  $C_{41}H_{83}NO_8P$ ).



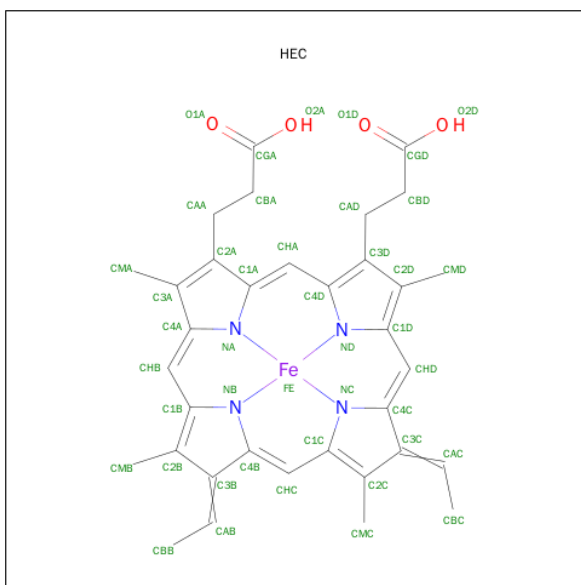
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	C	1	Total C N O P 49 39 1 8 1	0	0
15	C	1	Total C O P 21 12 8 1	0	0
15	E	1	Total C N O P 50 40 1 8 1	0	0
15	N	1	Total O P 5 4 1	0	0
15	P	1	Total C N O P 49 39 1 8 1	0	0
15	R	1	Total C N O P 50 40 1 8 1	0	0

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



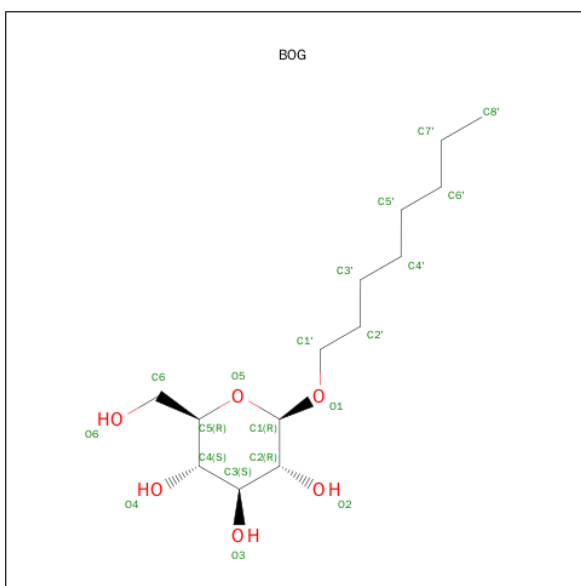
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	C	1	Total C O 6 3 3	0	0
16	P	1	Total C O 6 3 3	0	0

- 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 43	C 34	Fe 1	N 4	O 4	0	0
17	Q	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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



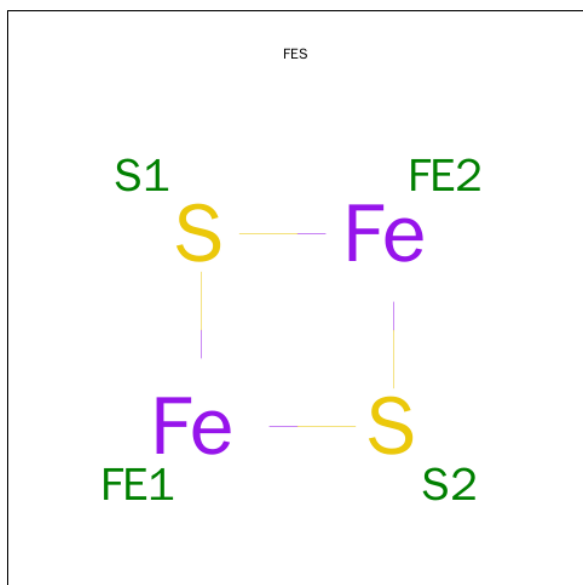
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	D	1	Total C O 20 14 6	0	0
18	D	1	Total C O 13 7 6	0	0

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

- Molecule 19 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



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

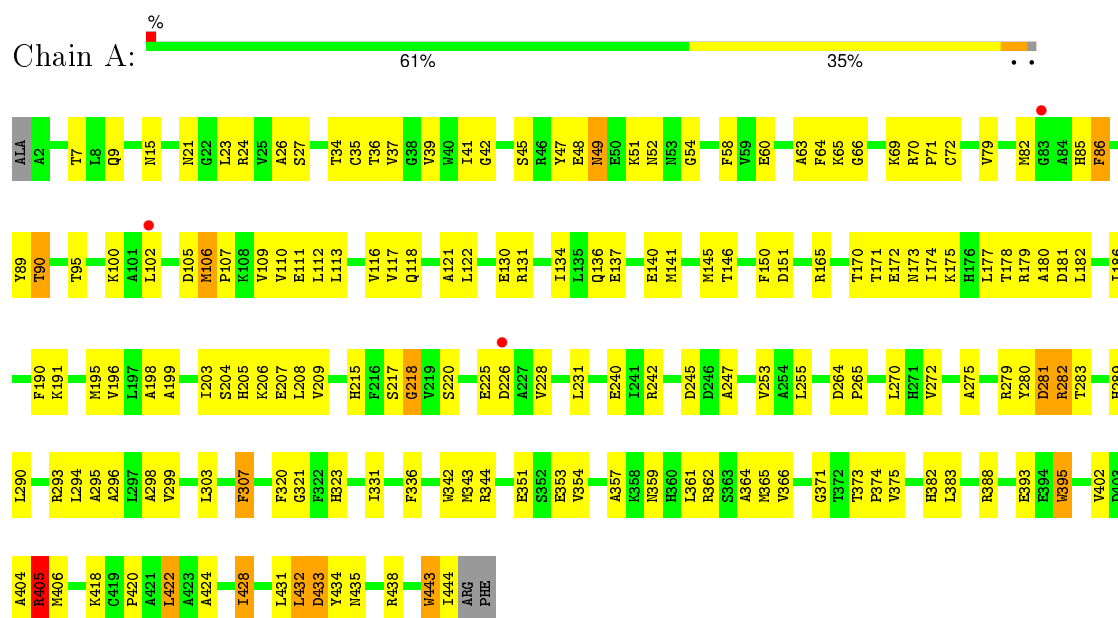
- Molecule 20 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	C	8	Total	O	0	0
			8	8		
20	E	1	Total	O	0	0
			1	1		
20	P	9	Total	O	0	0
			9	9		
20	R	1	Total	O	0	0
			1	1		

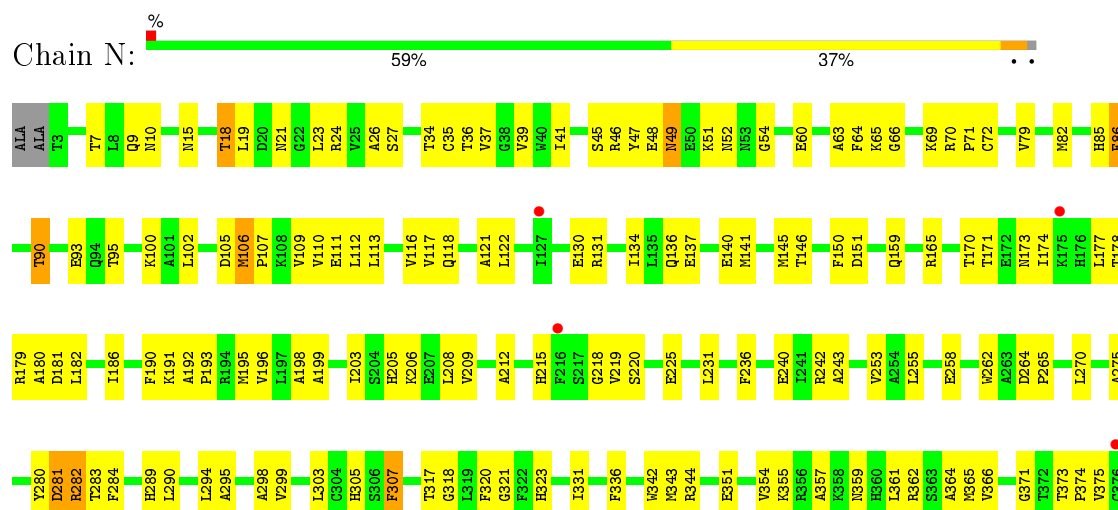
### 3 Residue-property plots

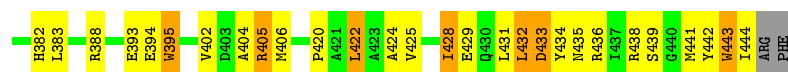
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN I, MITOCHONDRIAL

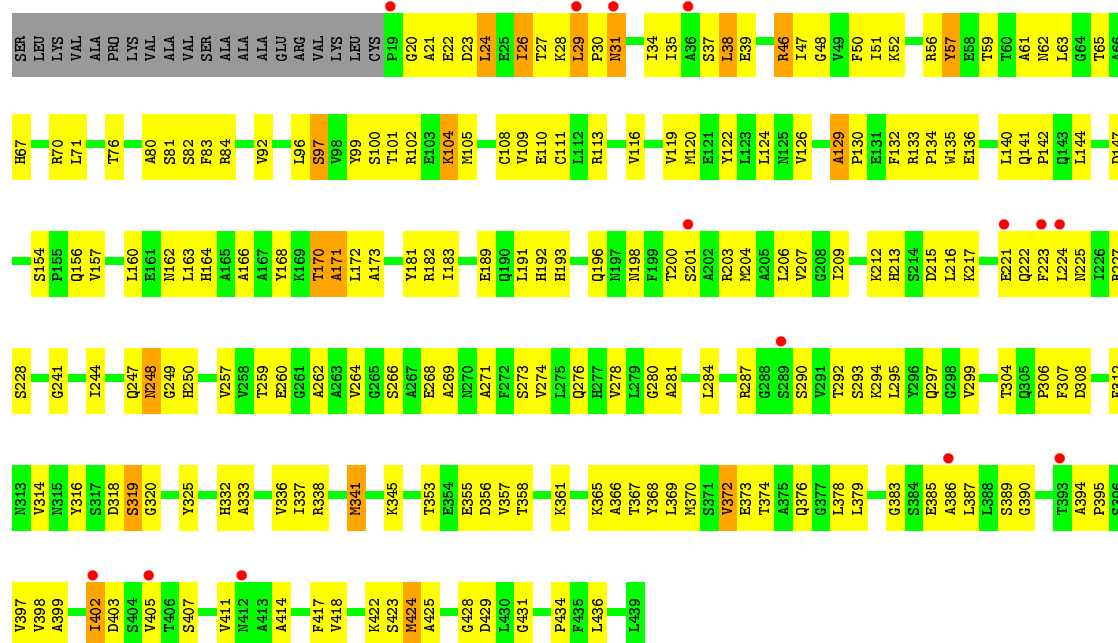


- Molecule 1: UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN I, MITOCHONDRIAL

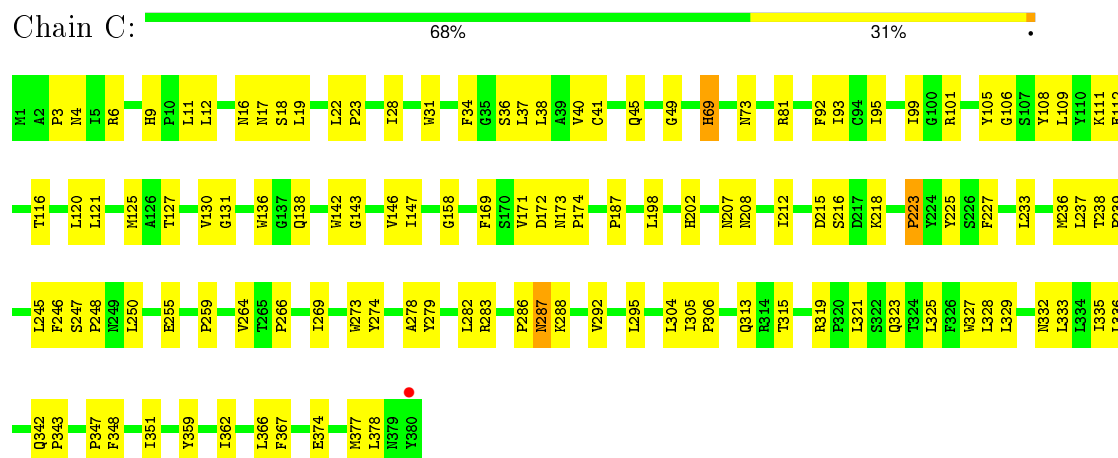




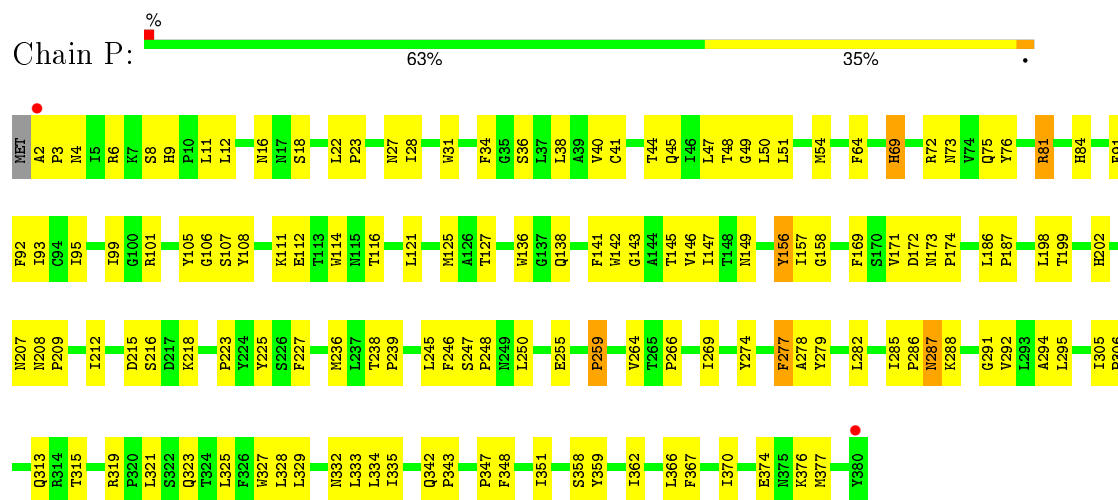
• Molecule 2: UBIQUINOL-CYTOCHROME-C REDUCTASE COMPLEX CORE PROTEIN 2, MITOCHONDRIAL



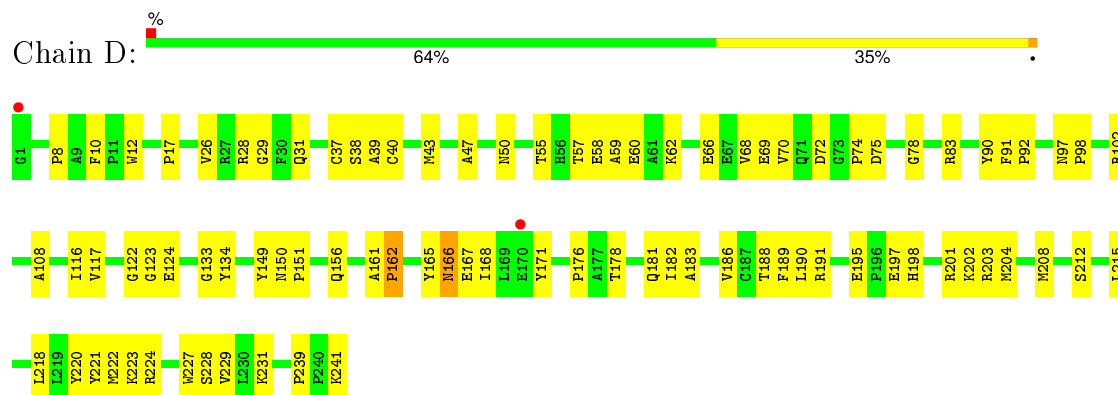
- Molecule 3: Cytochrome b



- Molecule 3: Cytochrome b

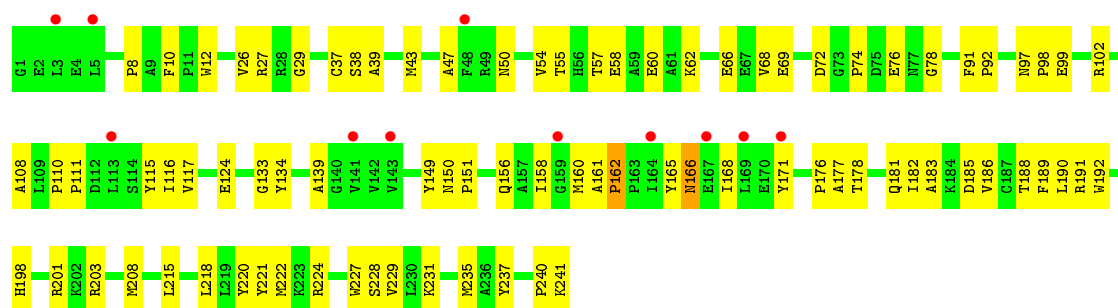


- Molecule 4: CYTOCHROME C1, HEME PROTEIN, MITOCHONDRIAL

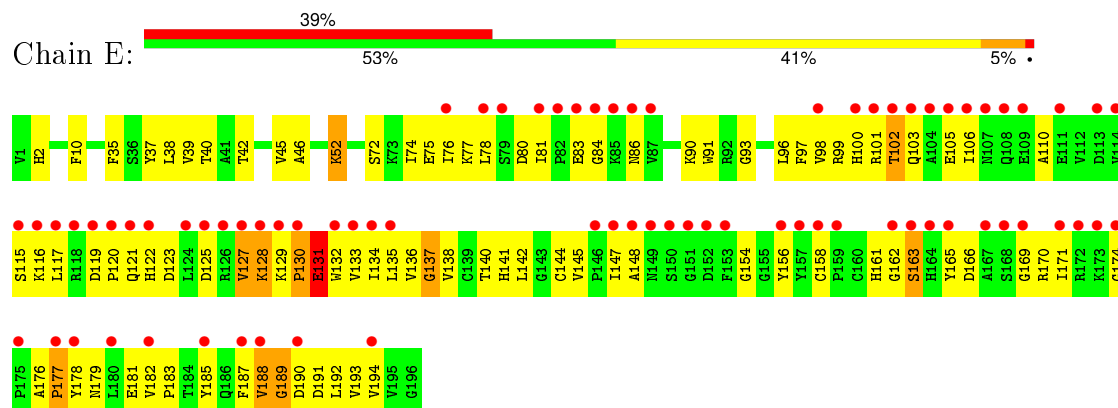


- Molecule 4: CYTOCHROME C1, HEME PROTEIN, MITOCHONDRIAL

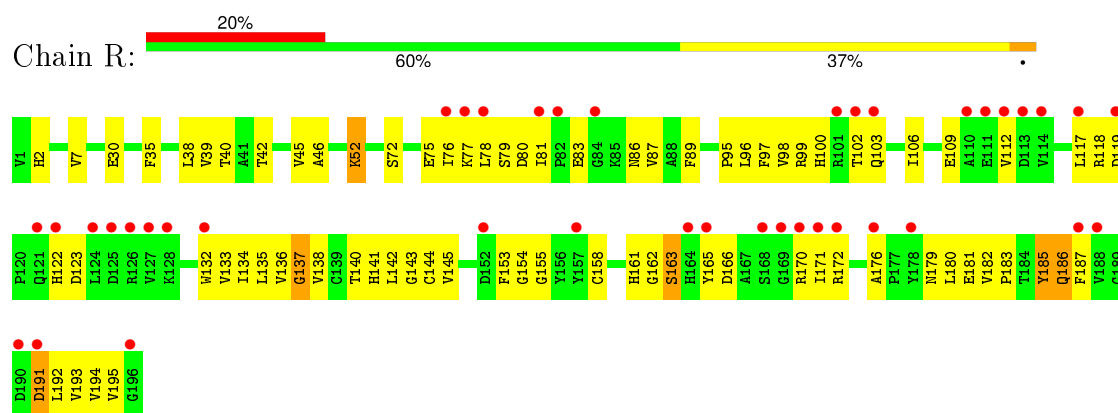




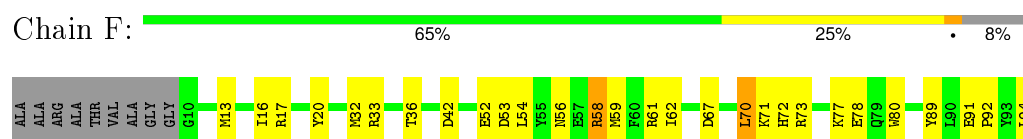
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial



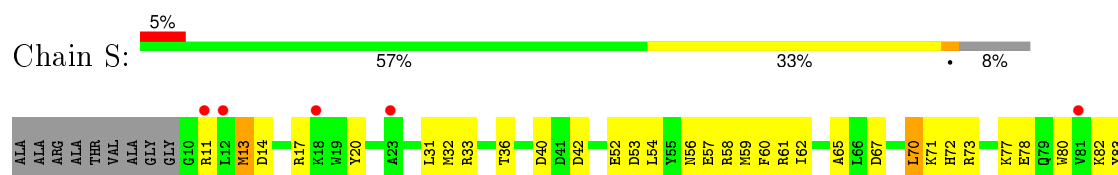
• Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial



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



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







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



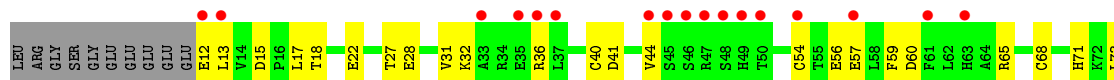
- Molecule 7: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX UBIQUINONE-BINDING PROTEIN QP-C



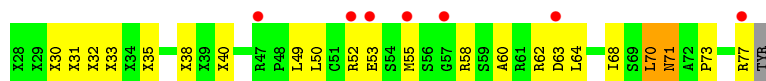
- Molecule 8: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 11 KDA PROTEIN



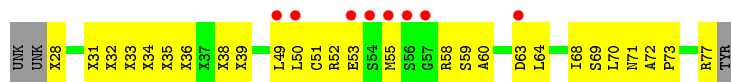
- Molecule 8: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 11 KDA PROTEIN




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



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




- Molecule 10: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 7.2 KDA PROTEIN

Chain J: 



- Molecule 10: UBIQUINOL-CYTOCHROME C REDUCTASE COMPLEX 7.2 KDA PROTEIN

Chain W: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	169.59Å 182.52Å 240.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.16 69.31 – 3.16	Depositor EDS
% Data completeness (in resolution range)	97.1 (20.00-3.16) 96.9 (69.31-3.16)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.00 (at 3.19Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.253 , 0.291 0.234 , 0.270	Depositor DCC
$R_{free}$ test set	2451 reflections (2.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	75.4	Xtriage
Anisotropy	0.738	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 72.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 123805 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	32608	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.98% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CDL, UQ, 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	0.48	0/3513	0.67	0/4760
1	N	0.46	0/3508	0.66	0/4753
2	B	0.41	0/3196	0.64	0/4334
2	O	0.44	0/3202	0.67	1/4343 (0.0%)
3	C	0.54	0/3119	0.69	0/4270
3	P	0.48	0/3114	0.65	0/4263
4	D	0.48	0/1956	0.66	1/2658 (0.0%)
4	Q	0.39	0/1956	0.63	1/2658 (0.0%)
5	E	0.40	0/1547	0.60	0/2103
5	R	0.39	0/1543	0.61	1/2098 (0.0%)
6	F	0.54	0/911	0.66	0/1219
6	S	0.44	0/911	0.62	0/1219
7	G	0.53	0/694	0.69	1/941 (0.1%)
7	T	0.46	0/684	0.66	1/929 (0.1%)
8	H	0.48	0/582	0.65	0/779
8	U	0.36	0/561	0.59	0/751
9	I	0.45	0/218	0.66	0/293
9	V	0.43	0/218	0.65	0/293
10	J	0.46	0/508	0.62	0/682
10	W	0.41	0/490	0.59	0/660
All	All	0.46	0/32431	0.65	6/44006 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	T	18	LEU	CA-CB-CG	5.82	128.69	115.30
4	D	133	GLY	N-CA-C	5.71	127.39	113.10
4	Q	133	GLY	N-CA-C	5.44	126.69	113.10
7	G	18	LEU	CA-CB-CG	5.37	127.65	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	R	143	GLY	N-CA-C	5.11	125.88	113.10
2	O	226	ILE	N-CA-C	-5.00	97.49	111.00

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3442	0	3354	153	0
1	N	3437	0	3349	155	0
2	B	3141	0	3142	215	0
2	O	3147	0	3146	215	0
3	C	3017	0	3063	108	0
3	P	3012	0	3058	126	0
4	D	1898	0	1846	71	0
4	Q	1898	0	1846	75	0
5	E	1513	0	1478	94	0
5	R	1509	0	1474	87	0
6	F	891	0	893	25	0
6	S	891	0	893	35	0
7	G	672	0	653	31	0
7	T	662	0	645	33	0
8	H	574	0	548	18	0
8	U	553	0	535	25	0
9	I	287	0	250	40	0
9	V	278	0	253	38	0
10	J	497	0	490	8	0
10	W	479	0	478	9	0
11	A	3	0	0	0	0
11	C	2	0	0	0	0
11	N	3	0	0	0	0
11	P	1	0	0	0	0
12	C	86	0	60	6	0
12	P	86	0	60	8	0
13	C	19	0	17	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	P	19	0	17	4	0
14	C	40	0	24	2	0
14	D	42	0	28	2	0
14	P	40	0	24	2	0
14	Q	42	0	28	3	0
15	C	70	0	85	2	0
15	E	50	0	77	1	0
15	N	5	0	0	0	0
15	P	49	0	72	2	0
15	R	50	0	77	0	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	1	0
18	D	33	0	39	1	0
18	P	12	0	11	1	0
18	Q	33	0	39	0	0
19	E	4	0	0	2	0
19	R	4	0	0	2	0
20	C	8	0	0	1	0
20	E	1	0	0	0	0
20	P	9	0	0	2	0
20	R	1	0	0	0	0
All	All	32608	0	32128	1415	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 22.

All (1415) 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	1.40	1.04
9:I:33:UNK:HG2	9:I:73:PRO:HB3	1.07	1.02
1:N:10:ASN:HD21	2:O:18:CYS:HB3	1.23	1.01
9:I:32:UNK:N	9:I:73:PRO:HG2	1.75	0.99
1:A:178:THR:HG22	1:A:180:ALA:H	1.27	0.99
2:B:353:THR:HG22	2:B:355:GLU:H	1.27	0.98
2:O:353:THR:HG22	2:O:355:GLU:H	1.26	0.97
1:N:178:THR:HG22	1:N:180:ALA:H	1.26	0.97
9:I:33:UNK:HG2	9:I:73:PRO:CB	1.95	0.96
2:B:124:LEU:HD11	2:B:223:PHE:HB3	1.46	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:238:THR:HB	3:P:239:PRO:HD3	1.48	0.95
1:N:106:MET:HG3	1:N:203:ILE:HD13	1.48	0.95
5:E:121:GLN:HG2	5:E:170:ARG:HD3	1.50	0.94
4:D:47:ALA:H	4:D:50:ASN:HD22	1.14	0.93
2:B:341:MET:HE1	2:B:417:PHE:HE2	1.31	0.92
4:Q:231:LYS:O	6:S:71:LYS:HE3	1.69	0.91
4:Q:47:ALA:H	4:Q:50:ASN:HD22	1.07	0.89
2:B:160:LEU:HD12	9:I:64:LEU:HD13	1.53	0.89
2:O:219:VAL:O	2:O:223:PHE:HB2	1.73	0.89
1:A:106:MET:HG3	1:A:203:ILE:HD13	1.53	0.88
3:C:238:THR:HB	3:C:239:PRO:HD3	1.55	0.88
2:B:76:THR:HG22	2:B:82:SER:H	1.39	0.88
5:E:81:ILE:HB	5:E:132:TRP:HH2	1.39	0.88
5:E:127:VAL:HG12	5:E:128:LYS:H	1.38	0.87
2:O:27:THR:HG22	2:O:28:LYS:H	1.37	0.86
2:O:37:SER:HB3	2:O:213:HIS:ND1	1.91	0.86
3:C:328:LEU:HD12	7:G:51:PRO:HB3	1.57	0.86
2:O:76:THR:HG22	2:O:82:SER:H	1.39	0.86
1:A:37:VAL:HG12	1:A:199:ALA:HB1	1.55	0.85
1:N:37:VAL:HG12	1:N:199:ALA:HB1	1.55	0.85
2:B:24:LEU:HD12	2:B:37:SER:O	1.76	0.85
2:B:47:ILE:HD13	2:B:120:MET:CE	2.07	0.85
9:I:33:UNK:CG	9:I:73:PRO:HB3	2.02	0.84
2:O:341:MET:HE1	2:O:417:PHE:HE2	1.42	0.84
2:O:248:ASN:HD22	2:O:249:GLY:N	1.75	0.83
2:B:168:TYR:HB2	2:B:173:ALA:HB2	1.59	0.83
5:E:90:LYS:HE3	5:E:93:GLY:HA2	1.60	0.83
1:A:242:ARG:HH12	1:A:432:LEU:HA	1.42	0.83
2:O:46:ARG:NH2	2:O:376:GLN:HG3	1.94	0.83
2:O:47:ILE:HD13	2:O:120:MET:HE2	1.60	0.83
2:O:221:GLU:HG3	2:O:222:GLN:H	1.42	0.83
2:O:51:ILE:HG12	2:O:204:MET:HG2	1.60	0.83
2:O:314:VAL:HG13	9:V:63:ASP:HB3	1.60	0.83
2:B:23:ASP:O	2:B:24:LEU:HB3	1.76	0.82
9:I:38:UNK:C	9:I:40:UNK:H	1.89	0.82
1:N:242:ARG:HH12	1:N:432:LEU:HA	1.43	0.82
3:P:212:ILE:HD12	6:S:62:ILE:HG23	1.60	0.82
2:B:248:ASN:HD22	2:B:249:GLY:N	1.76	0.82
4:D:231:LYS:O	6:F:71:LYS:HE3	1.79	0.82
2:B:157:VAL:HG23	9:I:64:LEU:HD21	1.59	0.82
3:P:328:LEU:HD12	7:T:51:PRO:HB3	1.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:127:THR:HG21	12:P:501:HEM:HBB2	1.62	0.81
5:E:166:ASP:OD2	5:E:170:ARG:HB2	1.81	0.81
2:O:154:SER:O	2:O:157:VAL:HG12	1.81	0.80
4:Q:218:LEU:HD11	5:R:42:THR:HG22	1.64	0.80
4:D:218:LEU:HD11	5:E:42:THR:HG22	1.64	0.79
2:O:96:LEU:HD13	2:O:109:VAL:HG12	1.61	0.79
2:O:27:THR:HG22	2:O:28:LYS:N	1.97	0.79
2:B:37:SER:HB3	2:B:213:HIS:ND1	1.97	0.79
2:O:168:TYR:HB2	2:O:173:ALA:HB2	1.64	0.79
1:A:60:GLU:OE2	1:A:90:THR:HG22	1.81	0.79
1:N:60:GLU:OE2	1:N:90:THR:HG22	1.83	0.79
2:O:24:LEU:HD12	2:O:37:SER:O	1.83	0.78
2:O:47:ILE:HD13	2:O:120:MET:CE	2.13	0.78
2:B:357:VAL:HG12	2:B:361:LYS:HE3	1.66	0.78
5:E:101:ARG:HA	5:E:105:GLU:OE1	1.84	0.78
1:N:105:ASP:O	1:N:109:VAL:HG23	1.85	0.78
2:O:357:VAL:HG12	2:O:361:LYS:HE3	1.66	0.77
2:O:160:LEU:HD12	9:V:64:LEU:HD13	1.67	0.77
5:E:83:GLU:HB3	5:E:102:THR:HG22	1.66	0.77
2:B:76:THR:CG2	2:B:82:SER:H	1.97	0.77
5:R:166:ASP:OD2	5:R:170:ARG:HB2	1.84	0.77
2:B:144:LEU:HB2	2:B:183:ILE:HD12	1.66	0.76
1:N:49:ASN:ND2	1:N:51:LYS:H	1.83	0.76
2:B:274:VAL:O	2:B:278:VAL:HG23	1.86	0.76
3:C:127:THR:HG21	12:C:501:HEM:HBB2	1.67	0.76
9:I:70:LEU:HD23	9:I:71:ASN:H	1.50	0.76
3:C:278:ALA:HB1	3:C:295:LEU:CD1	2.16	0.76
2:O:76:THR:CG2	2:O:82:SER:H	2.00	0.75
2:B:47:ILE:HD13	2:B:120:MET:HE2	1.67	0.75
2:O:47:ILE:HD11	2:O:116:VAL:HG13	1.66	0.75
2:B:27:THR:HG22	2:B:28:LYS:N	2.02	0.75
2:B:287:ARG:HB3	9:I:53:GLU:HG3	1.68	0.75
2:B:71:LEU:HD12	2:B:144:LEU:HD23	1.67	0.74
2:B:57:TYR:CE2	2:B:203:ARG:NH2	2.54	0.74
2:B:51:ILE:HG12	2:B:204:MET:HG2	1.68	0.74
7:T:50:PRO:HB2	7:T:51:PRO:CD	2.17	0.74
2:O:338:ARG:HH11	2:O:338:ARG:HG3	1.50	0.74
2:O:57:TYR:CE2	2:O:203:ARG:NH2	2.54	0.74
5:E:136:VAL:HG23	5:E:183:PRO:HD3	1.69	0.74
2:B:62:ASN:O	2:B:65:THR:HG22	1.88	0.74
2:B:27:THR:HG22	2:B:28:LYS:H	1.52	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:338:ARG:HG3	2:B:338:ARG:HH11	1.52	0.73
5:R:117:LEU:HD21	5:R:172:ARG:NH1	2.02	0.73
1:N:443:TRP:CE3	1:N:443:TRP:HA	2.23	0.73
1:A:49:ASN:ND2	1:A:51:LYS:H	1.85	0.73
2:O:422:LYS:O	2:O:436:LEU:HD21	1.88	0.73
2:B:154:SER:O	2:B:157:VAL:HG12	1.88	0.73
2:B:63:LEU:HB2	2:B:182:ARG:HD3	1.71	0.73
2:B:47:ILE:HD11	2:B:116:VAL:HG13	1.69	0.73
3:P:106:GLY:HA2	3:P:108:TYR:CE2	2.24	0.73
2:O:71:LEU:HD12	2:O:144:LEU:HD23	1.71	0.73
1:A:23:LEU:HD23	1:A:24:ARG:N	2.03	0.73
2:B:124:LEU:HD11	2:B:223:PHE:CB	2.18	0.73
2:O:144:LEU:HB2	2:O:183:ILE:HD12	1.69	0.72
3:C:342:GLN:HE21	3:C:343:PRO:HD2	1.54	0.72
2:O:274:VAL:O	2:O:278:VAL:HG23	1.89	0.72
3:C:212:ILE:HD12	6:F:62:ILE:HG23	1.72	0.72
4:Q:139:ALA:HB3	8:U:54:CYS:SG	2.29	0.72
1:A:37:VAL:HG12	1:A:199:ALA:CB	2.18	0.72
1:A:7:THR:HG21	2:B:113:ARG:HD2	1.71	0.72
5:E:119:ASP:HB3	5:E:179:ASN:HD21	1.55	0.72
2:O:62:ASN:O	2:O:65:THR:HG22	1.90	0.71
7:G:50:PRO:HB2	7:G:51:PRO:CD	2.20	0.71
3:C:9:HIS:HD2	3:C:12:LEU:H	1.38	0.71
3:P:22:LEU:HD21	13:P:3002:UQ:HM32	1.70	0.71
2:B:314:VAL:HG13	9:I:63:ASP:HB3	1.70	0.71
4:D:222:MET:HE1	5:E:40:THR:HG23	1.71	0.71
7:G:29:ILE:O	7:G:33:ALA:HB3	1.91	0.71
1:A:443:TRP:CE3	1:A:443:TRP:HA	2.23	0.71
1:A:140:GLU:OE2	9:I:50:LEU:N	2.19	0.71
3:C:236:MET:O	3:C:239:PRO:HD2	1.91	0.70
1:N:37:VAL:HG12	1:N:199:ALA:CB	2.21	0.70
3:P:92:PHE:HA	3:P:95:ILE:HG22	1.73	0.70
4:D:97:ASN:HB2	4:D:98:PRO:HD2	1.73	0.70
9:V:31:UNK:C	9:V:73:PRO:HG2	2.21	0.70
3:C:169:PHE:HE1	5:R:72:SER:HA	1.57	0.70
2:B:46:ARG:NH2	2:B:376:GLN:HG3	2.07	0.70
5:R:136:VAL:HG23	5:R:183:PRO:HD3	1.71	0.70
1:N:281:ASP:O	1:N:283:THR:N	2.24	0.70
2:O:181:TYR:CE1	2:O:182:ARG:HG3	2.26	0.70
1:A:85:HIS:CD2	2:B:284:LEU:HD22	2.26	0.70
1:A:130:GLU:O	1:A:134:ILE:HG13	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:9:HIS:HD2	3:P:12:LEU:H	1.40	0.69
2:B:96:LEU:HD13	2:B:109:VAL:HG12	1.73	0.69
3:P:278:ALA:HB1	3:P:295:LEU:CD1	2.22	0.69
1:A:206:LYS:HA	1:A:209:VAL:HG12	1.74	0.69
1:A:281:ASP:O	1:A:283:THR:N	2.26	0.69
2:B:209:ILE:HD13	2:B:378:LEU:HD23	1.75	0.69
3:P:342:GLN:HE21	3:P:343:PRO:HD2	1.56	0.69
4:Q:47:ALA:H	4:Q:50:ASN:ND2	1.87	0.69
5:R:83:GLU:HA	5:R:100:HIS:HB3	1.75	0.69
5:E:86:ASN:HD22	5:E:148:ALA:HB2	1.56	0.69
4:Q:97:ASN:HB2	4:Q:98:PRO:HD2	1.74	0.69
2:B:181:TYR:CE1	2:B:182:ARG:HG3	2.28	0.68
1:N:443:TRP:HE3	1:N:443:TRP:HA	1.56	0.68
2:B:399:ALA:O	2:B:402:ILE:HG22	1.94	0.68
5:R:83:GLU:HG3	5:R:100:HIS:CE1	2.29	0.68
7:T:29:ILE:O	7:T:33:ALA:HB3	1.93	0.68
1:N:112:LEU:O	1:N:116:VAL:HG23	1.94	0.68
2:O:361:LYS:HD3	2:O:403:ASP:HA	1.74	0.67
2:B:31:ASN:N	2:B:31:ASN:HD22	1.90	0.67
4:D:181:GLN:HA	8:H:77:LEU:HD22	1.76	0.67
1:A:178:THR:HB	1:A:181:ASP:OD1	1.94	0.67
5:E:81:ILE:HB	5:E:132:TRP:CH2	2.26	0.67
2:O:337:ILE:HD12	2:O:434:PRO:HD2	1.74	0.67
1:N:130:GLU:O	1:N:134:ILE:HG13	1.94	0.67
2:O:248:ASN:HD21	2:O:428:GLY:HA2	1.57	0.67
1:A:443:TRP:HE3	1:A:443:TRP:HA	1.56	0.67
5:E:76:ILE:HD13	5:E:98:VAL:HG21	1.76	0.67
2:B:248:ASN:HD22	2:B:248:ASN:C	1.94	0.67
8:U:18:THR:O	8:U:22:GLU:HG3	1.94	0.67
2:O:47:ILE:HG21	2:O:120:MET:HE1	1.77	0.67
4:D:229:VAL:HG23	7:G:20:PRO:HG3	1.76	0.67
2:B:422:LYS:O	2:B:436:LEU:HD21	1.95	0.67
5:R:78:LEU:HB3	5:R:132:TRP:CZ2	2.30	0.67
1:A:111:GLU:HG3	1:A:215:HIS:CD2	2.28	0.67
5:E:78:LEU:HD12	5:E:190:ASP:O	1.95	0.67
1:N:7:THR:HG21	2:O:113:ARG:HD2	1.77	0.66
5:E:121:GLN:HG2	5:E:170:ARG:CD	2.25	0.66
3:P:199:THR:HA	18:P:2010:BOG:O1	1.95	0.66
7:T:41:PHE:O	7:T:45:VAL:HG23	1.94	0.66
2:B:76:THR:HG22	2:B:81:SER:HA	1.78	0.66
2:O:71:LEU:CD1	2:O:144:LEU:HD23	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:286:PRO:O	3:C:287:ASN:HB2	1.94	0.66
1:N:85:HIS:CD2	2:O:284:LEU:HD22	2.29	0.66
5:R:102:THR:O	5:R:106:ILE:HG13	1.95	0.66
5:R:78:LEU:HD13	5:R:132:TRP:NE1	2.11	0.66
2:O:248:ASN:HD22	2:O:248:ASN:C	1.94	0.66
3:C:92:PHE:HA	3:C:95:ILE:HG22	1.77	0.66
3:P:325:LEU:HD21	3:P:366:LEU:HB3	1.77	0.66
3:P:121:LEU:O	3:P:125:MET:HG3	1.96	0.66
2:O:63:LEU:HB2	2:O:182:ARG:HD3	1.76	0.65
2:B:394:ALA:HB3	2:B:397:VAL:HG23	1.76	0.65
2:O:27:THR:CG2	2:O:28:LYS:H	2.08	0.65
2:B:130:PRO:HB2	2:B:132:PHE:CE2	2.32	0.65
10:W:49:GLY:N	10:W:54:HIS:ND1	2.45	0.65
1:A:336:PHE:CE2	3:C:4:ASN:HB3	2.31	0.65
5:R:119:ASP:HB3	5:R:179:ASN:ND2	2.11	0.65
7:T:72:LYS:HE2	8:U:57:GLU:OE1	1.96	0.65
2:O:314:VAL:CG1	9:V:63:ASP:HB3	2.24	0.65
1:N:146:THR:HG23	1:N:323:HIS:CE1	2.31	0.65
3:P:212:ILE:CD1	6:S:62:ILE:HG23	2.26	0.65
1:N:298:ALA:HA	1:N:303:LEU:HB2	1.78	0.65
1:A:146:THR:HG23	1:A:323:HIS:CE1	2.31	0.65
1:N:23:LEU:HD23	1:N:24:ARG:N	2.11	0.65
7:T:73:ASN:HD21	7:T:75:ALA:HB3	1.61	0.65
5:R:81:ILE:HG22	5:R:100:HIS:HB2	1.79	0.64
1:A:331:ILE:HG21	1:A:431:LEU:HB2	1.79	0.64
1:N:382:HIS:HB3	1:N:388:ARG:O	1.97	0.64
5:R:136:VAL:HG21	5:R:181:GLU:OE1	1.97	0.64
5:R:134:ILE:HD12	5:R:185:TYR:CD1	2.32	0.64
1:N:321:GLY:HA2	1:N:342:TRP:HZ2	1.62	0.64
5:E:101:ARG:HG2	5:E:105:GLU:OE2	1.98	0.64
2:O:273:SER:O	2:O:276:GLN:HB3	1.98	0.64
2:B:341:MET:HE1	2:B:417:PHE:CE2	2.23	0.64
1:N:402:VAL:HG22	1:N:406:MET:CE	2.28	0.64
3:P:207:ASN:ND2	3:P:208:ASN:H	1.96	0.64
7:G:73:ASN:HD21	7:G:75:ALA:HB3	1.63	0.64
10:J:49:GLY:N	10:J:54:HIS:ND1	2.46	0.64
1:N:111:GLU:HG3	1:N:215:HIS:CD2	2.33	0.64
5:R:186:GLN:O	5:R:193:VAL:HG23	1.98	0.64
1:A:105:ASP:O	1:A:109:VAL:HG23	1.97	0.63
1:A:64:PHE:HE2	1:A:86:PHE:CZ	2.16	0.63
3:C:278:ALA:HB1	3:C:295:LEU:HD12	1.78	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:399:ALA:O	2:O:402:ILE:HG22	1.97	0.63
4:D:57:THR:HB	4:D:60:GLU:HG3	1.81	0.63
2:B:341:MET:CE	2:B:417:PHE:HE2	2.05	0.63
1:A:281:ASP:CG	9:I:33:UNK:HB2	2.19	0.63
3:P:105:TYR:HA	3:P:315:THR:HG22	1.80	0.63
1:A:321:GLY:HA2	1:A:342:TRP:HZ2	1.63	0.63
1:N:331:ILE:HG21	1:N:431:LEU:HB2	1.81	0.63
1:A:36:THR:HG21	1:A:373:THR:HA	1.81	0.63
2:B:206:LEU:HG	2:B:216:LEU:HD11	1.81	0.63
3:P:138:GLN:OE1	3:P:138:GLN:HA	1.99	0.63
1:A:191:LYS:CA	1:A:195:MET:HE2	2.29	0.62
1:N:336:PHE:CE2	3:P:4:ASN:HB3	2.35	0.62
2:O:76:THR:HG22	2:O:81:SER:HA	1.82	0.62
2:O:394:ALA:HB3	2:O:397:VAL:HG23	1.82	0.62
5:R:118:ARG:HB2	5:R:118:ARG:NH1	2.15	0.62
7:G:41:PHE:O	7:G:45:VAL:HG23	1.98	0.62
2:B:122:TYR:O	2:B:126:VAL:HG23	2.00	0.62
1:N:343:MET:HB3	1:N:444:ILE:HA	1.81	0.62
1:N:106:MET:HG3	1:N:203:ILE:CD1	2.27	0.62
3:C:105:TYR:HA	3:C:315:THR:HG22	1.80	0.62
2:B:76:THR:HG22	2:B:82:SER:N	2.12	0.62
1:A:240:GLU:OE1	1:A:434:TYR:HB2	1.99	0.62
1:N:165:ARG:HG3	1:N:165:ARG:HH11	1.65	0.62
2:O:399:ALA:HA	2:O:402:ILE:HG22	1.82	0.62
2:B:132:PHE:CE1	2:B:191:LEU:HB3	2.35	0.62
1:A:112:LEU:O	1:A:116:VAL:HG23	2.00	0.62
2:O:361:LYS:O	2:O:365:LYS:HG3	1.99	0.61
8:H:18:THR:O	8:H:22:GLU:HG3	1.99	0.61
2:O:345:LYS:HG2	2:O:418:VAL:CG1	2.30	0.61
1:A:371:GLY:O	1:A:375:VAL:HG23	2.00	0.61
4:D:62:LYS:O	4:D:66:GLU:HG3	2.00	0.61
2:O:341:MET:CE	2:O:417:PHE:HE2	2.11	0.61
1:N:270:LEU:HD22	1:N:320:PHE:CE1	2.35	0.61
3:P:335:ILE:HD13	7:T:58:LEU:HD23	1.81	0.61
2:B:337:ILE:HD12	2:B:434:PRO:HD2	1.80	0.61
8:H:12:GLU:HG2	8:H:13:LEU:N	2.15	0.61
1:N:371:GLY:O	1:N:375:VAL:HG23	2.00	0.61
2:O:353:THR:HB	2:O:356:ASP:OD1	2.00	0.61
5:E:72:SER:HA	3:P:169:PHE:HE1	1.64	0.61
6:F:91:GLU:HB3	6:F:92:PRO:HD3	1.82	0.61
6:S:13:MET:O	6:S:17:ARG:HG3	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:359:ASN:HD22	2:O:92:VAL:HA	1.65	0.61
5:E:137:GLY:O	5:E:145:VAL:HG13	2.00	0.61
5:E:135:LEU:HD11	5:E:169:GLY:HA3	1.83	0.61
9:I:31:UNK:C	9:I:73:PRO:HG2	2.30	0.61
2:B:332:HIS:O	2:B:336:VAL:HG23	2.01	0.61
4:Q:76:GLU:CD	4:Q:76:GLU:H	2.03	0.61
3:P:236:MET:O	3:P:239:PRO:HD2	2.01	0.61
4:Q:62:LYS:O	4:Q:66:GLU:HG3	2.01	0.61
4:Q:171:TYR:OH	4:Q:182:ILE:HA	2.01	0.60
5:E:142:LEU:HD12	5:E:161:HIS:CE1	2.36	0.60
9:I:70:LEU:HD23	9:I:71:ASN:N	2.16	0.60
8:U:12:GLU:HG2	8:U:13:LEU:H	1.66	0.60
1:A:282:ARG:HH21	9:I:35:UNK:HA	1.65	0.60
1:A:281:ASP:OD1	9:I:33:UNK:HB2	2.02	0.60
2:B:71:LEU:CD1	2:B:144:LEU:HD23	2.30	0.60
2:O:209:ILE:HD13	2:O:378:LEU:HD23	1.83	0.60
1:N:424:ALA:HB1	1:N:428:ILE:HG21	1.83	0.60
2:O:46:ARG:HH22	2:O:376:GLN:HG3	1.67	0.60
2:B:147:ASP:OD1	9:I:68:ILE:HD11	2.01	0.60
4:Q:181:GLN:HA	8:U:77:LEU:HD22	1.84	0.60
3:C:313:GLN:NE2	6:F:36:THR:OG1	2.34	0.60
1:N:206:LYS:HA	1:N:209:VAL:HG12	1.83	0.60
2:B:248:ASN:HD21	2:B:428:GLY:HA2	1.66	0.60
2:B:132:PHE:CD1	2:B:191:LEU:HB3	2.37	0.60
2:B:333:ALA:O	2:B:337:ILE:HG13	2.01	0.60
3:P:313:GLN:NE2	6:S:36:THR:OG1	2.33	0.60
1:A:178:THR:HG22	1:A:180:ALA:N	2.09	0.60
1:N:63:ALA:O	1:N:116:VAL:HG13	2.02	0.60
3:C:106:GLY:HA2	3:C:108:TYR:CE2	2.36	0.60
6:F:42:ASP:OD1	6:F:101:ARG:NH1	2.34	0.60
5:E:106:ILE:O	5:E:110:ALA:HB3	2.02	0.60
4:D:171:TYR:OH	4:D:182:ILE:HA	2.01	0.60
1:N:64:PHE:HE2	1:N:86:PHE:CZ	2.20	0.60
2:B:31:ASN:ND2	2:B:31:ASN:H	2.00	0.60
1:A:402:VAL:HG22	1:A:406:MET:CE	2.31	0.59
1:N:131:ARG:NH2	1:N:177:LEU:O	2.35	0.59
3:P:286:PRO:O	3:P:287:ASN:HB2	2.02	0.59
1:A:280:TYR:CG	1:A:281:ASP:N	2.70	0.59
4:D:218:LEU:HD11	5:E:42:THR:CG2	2.32	0.59
2:O:402:ILE:HD13	2:O:402:ILE:C	2.23	0.59
1:A:402:VAL:HA	1:A:406:MET:CE	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:138:GLN:OE1	3:C:138:GLN:HA	2.00	0.59
1:A:298:ALA:HA	1:A:303:LEU:HB2	1.84	0.59
5:E:45:VAL:HG13	10:J:28:ALA:HA	1.85	0.59
5:E:101:ARG:HB2	5:E:131:GLU:HA	1.82	0.59
2:B:223:PHE:O	2:B:225:ASN:HB2	2.03	0.59
2:O:76:THR:HG22	2:O:82:SER:N	2.12	0.59
5:E:99:ARG:HB3	5:E:133:VAL:CG1	2.32	0.59
1:N:134:ILE:HG21	1:N:174:ILE:HD13	1.85	0.59
2:O:122:TYR:O	2:O:126:VAL:HG23	2.03	0.59
2:B:294:LYS:HE3	2:B:356:ASP:OD2	2.03	0.59
2:B:361:LYS:HD3	2:B:403:ASP:HA	1.83	0.59
3:P:245:LEU:O	4:Q:201:ARG:HD3	2.02	0.59
1:N:15:ASN:O	1:N:26:ALA:HA	2.02	0.59
2:O:372:VAL:O	2:O:372:VAL:HG12	2.01	0.59
1:N:255:LEU:HD12	1:N:422:LEU:HB2	1.84	0.59
3:C:325:LEU:HD21	3:C:366:LEU:HB3	1.83	0.59
5:R:99:ARG:HB3	5:R:133:VAL:CG1	2.33	0.59
2:O:56:ARG:HG3	2:O:56:ARG:HH11	1.67	0.59
2:B:399:ALA:HA	2:B:402:ILE:HG22	1.84	0.59
3:C:143:GLY:O	3:C:147:ILE:HG12	2.02	0.59
2:B:264:VAL:HG23	2:B:316:TYR:C	2.23	0.59
2:O:294:LYS:HE3	2:O:356:ASP:OD2	2.02	0.59
7:T:73:ASN:ND2	7:T:75:ALA:HB3	2.16	0.59
2:O:333:ALA:O	2:O:337:ILE:HG13	2.03	0.58
7:T:72:LYS:HG2	8:U:56:GLU:OE2	2.02	0.58
2:O:345:LYS:HG2	2:O:418:VAL:HG13	1.85	0.58
1:N:170:THR:HG22	1:N:171:THR:N	2.18	0.58
5:E:119:ASP:HB3	5:E:179:ASN:ND2	2.16	0.58
3:C:9:HIS:CD2	3:C:12:LEU:H	2.20	0.58
2:B:100:SER:HB2	2:B:105:MET:HG2	1.85	0.58
3:C:279:TYR:CE2	3:C:283:ARG:HD3	2.39	0.58
2:B:56:ARG:HG3	2:B:56:ARG:HH11	1.68	0.58
2:B:361:LYS:O	2:B:365:LYS:HG3	2.02	0.58
1:N:136:GLN:OE1	9:V:50:LEU:HD13	2.03	0.58
2:B:96:LEU:HD12	2:B:97:SER:N	2.19	0.58
5:E:136:VAL:O	5:E:138:VAL:N	2.31	0.58
5:E:141:HIS:O	5:E:142:LEU:HD23	2.04	0.58
1:N:36:THR:HG21	1:N:373:THR:HA	1.85	0.58
2:B:372:VAL:O	2:B:372:VAL:HG12	2.03	0.58
1:A:382:HIS:HB3	1:A:388:ARG:O	2.03	0.58
1:N:37:VAL:HG23	1:N:113:LEU:HD11	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:45:GLN:CB	12:C:501:HEM:HAB	2.34	0.58
9:V:33:UNK:HA	9:V:73:PRO:HG3	1.86	0.58
4:Q:8:PRO:HG2	4:Q:10:PHE:CE1	2.37	0.58
2:O:248:ASN:ND2	2:O:250:HIS:H	2.01	0.58
1:A:424:ALA:HB1	1:A:428:ILE:HG21	1.86	0.58
2:O:241:GLY:HA2	2:O:423:SER:HB3	1.85	0.58
2:O:99:TYR:HE1	2:O:108:CYS:SG	2.27	0.58
5:E:127:VAL:HG12	5:E:128:LYS:N	2.15	0.58
4:Q:139:ALA:HB2	8:U:41:ASP:HA	1.86	0.58
2:O:27:THR:CG2	2:O:28:LYS:N	2.67	0.58
2:O:52:LYS:O	2:O:203:ARG:NH2	2.37	0.58
3:C:34:PHE:HB2	20:C:381:HOH:O	2.04	0.58
5:E:84:GLY:N	5:E:102:THR:HG23	2.19	0.57
3:P:9:HIS:CD2	3:P:12:LEU:H	2.22	0.57
8:U:17:LEU:HD13	8:U:73:LEU:HD22	1.86	0.57
1:N:106:MET:O	1:N:110:VAL:HG23	2.04	0.57
1:N:395:TRP:HA	1:N:395:TRP:CE3	2.39	0.57
2:O:332:HIS:O	2:O:336:VAL:HG23	2.03	0.57
4:Q:240:PRO:HD3	7:T:12:HIS:CE1	2.39	0.57
2:O:100:SER:CB	2:O:105:MET:HG2	2.34	0.57
2:B:71:LEU:HD23	9:I:68:ILE:HG13	1.85	0.57
2:B:31:ASN:HD22	2:B:31:ASN:H	1.52	0.57
1:A:137:GLU:O	1:A:141:MET:HG3	2.04	0.57
2:B:290:SER:O	2:B:297:GLN:HG2	2.04	0.57
2:O:338:ARG:NH1	2:O:338:ARG:HG3	2.19	0.57
2:O:248:ASN:ND2	2:O:428:GLY:HA2	2.18	0.57
2:O:128:THR:HG21	2:O:224:LEU:HD22	1.86	0.57
4:Q:57:THR:HB	4:Q:60:GLU:HG3	1.86	0.57
5:E:190:ASP:C	5:E:192:LEU:H	2.07	0.57
2:B:353:THR:HB	2:B:356:ASP:OD1	2.04	0.57
9:V:70:LEU:CD2	9:V:71:ASN:OD1	2.53	0.57
1:N:90:THR:HB	1:N:95:THR:HG23	1.86	0.57
2:O:147:ASP:OD1	9:V:68:ILE:HD11	2.05	0.57
5:R:78:LEU:HD11	5:R:187:PHE:CE1	2.39	0.57
5:E:130:PRO:HG2	5:E:131:GLU:OE2	2.04	0.57
2:B:402:ILE:HD13	2:B:402:ILE:C	2.24	0.57
2:B:46:ARG:HD2	2:B:110:GLU:HG2	1.86	0.57
2:O:47:ILE:HG22	2:O:48:GLY:N	2.19	0.57
3:P:95:ILE:HD13	3:P:121:LEU:HD13	1.87	0.57
1:A:275:ALA:HB3	1:A:357:ALA:HB1	1.86	0.57
7:G:49:ALA:HB3	7:G:50:PRO:HD3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:27:THR:CG2	2:B:28:LYS:H	2.18	0.57
5:E:76:ILE:CD1	5:E:98:VAL:HG21	2.35	0.57
5:R:78:LEU:HD11	5:R:187:PHE:HE1	1.69	0.57
7:G:73:ASN:ND2	7:G:75:ALA:HB3	2.20	0.57
2:B:241:GLY:HA2	2:B:423:SER:HB3	1.87	0.57
5:R:45:VAL:HG13	10:W:28:ALA:HA	1.87	0.57
5:E:147:ILE:O	5:E:156:TYR:HA	2.05	0.57
4:Q:218:LEU:CD1	5:R:42:THR:HG22	2.34	0.56
9:V:70:LEU:HD23	9:V:71:ASN:OD1	2.05	0.56
2:B:38:LEU:HD12	2:B:38:LEU:C	2.24	0.56
2:B:46:ARG:HG3	2:B:379:LEU:HD22	1.87	0.56
3:P:215:ASP:HA	3:P:218:LYS:HE2	1.87	0.56
12:P:502:HEM:HBD1	20:P:386:HOH:O	2.04	0.56
3:P:238:THR:HB	3:P:239:PRO:CD	2.30	0.56
2:B:35:ILE:O	2:B:213:HIS:HE1	1.87	0.56
1:A:85:HIS:NE2	2:B:284:LEU:HD22	2.21	0.56
2:O:306:PRO:HB3	9:V:52:ARG:N	2.21	0.56
1:N:182:LEU:O	1:N:186:ILE:HG13	2.05	0.56
2:B:248:ASN:ND2	2:B:250:HIS:H	2.03	0.56
2:B:31:ASN:N	2:B:31:ASN:ND2	2.53	0.56
4:D:218:LEU:CD1	5:E:42:THR:HG22	2.34	0.56
5:R:122:HIS:CD2	5:R:123:ASP:H	2.24	0.56
5:R:170:ARG:HA	5:R:179:ASN:HB3	1.86	0.56
1:N:240:GLU:OE1	1:N:434:TYR:HB2	2.04	0.56
2:B:212:LYS:HB3	2:B:215:ASP:OD2	2.05	0.56
4:Q:149:TYR:CE1	4:Q:156:GLN:HB3	2.41	0.56
4:Q:139:ALA:CB	8:U:41:ASP:HA	2.35	0.56
1:N:402:VAL:HA	1:N:406:MET:CE	2.35	0.56
3:P:216:SER:HB3	6:S:59:MET:CE	2.35	0.56
5:R:75:GLU:HB3	5:R:194:VAL:HG22	1.86	0.56
1:N:275:ALA:HB3	1:N:357:ALA:HB1	1.88	0.56
4:D:149:TYR:CE1	4:D:156:GLN:HB3	2.40	0.56
2:B:47:ILE:HD11	2:B:116:VAL:CG1	2.36	0.56
2:B:357:VAL:CG1	2:B:361:LYS:HE3	2.35	0.56
3:C:37:LEU:O	3:C:41:CYS:HB2	2.05	0.56
3:C:245:LEU:O	4:D:201:ARG:HD3	2.06	0.56
3:P:142:TRP:O	3:P:146:VAL:HG23	2.05	0.56
2:B:395:PRO:HA	2:B:398:VAL:HG12	1.88	0.56
2:O:338:ARG:O	2:O:341:MET:HB2	2.06	0.56
5:R:109:GLU:CG	5:R:123:ASP:HB2	2.36	0.56
10:W:58:LYS:HB2	10:W:59:TYR:CE1	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:377:MET:HE2	6:F:20:TYR:CG	2.41	0.56
1:N:39:VAL:HG11	1:N:117:VAL:HG11	1.88	0.56
2:B:385:GLU:O	2:B:387:LEU:N	2.39	0.56
7:T:72:LYS:CE	8:U:57:GLU:OE1	2.53	0.56
2:B:100:SER:CB	2:B:105:MET:HG2	2.36	0.56
1:A:433:ASP:OD2	1:A:435:ASN:HB2	2.06	0.56
2:B:257:VAL:HG22	2:B:424:MET:HG3	1.88	0.56
2:B:338:ARG:HG3	2:B:338:ARG:NH1	2.20	0.55
6:S:77:LYS:HA	6:S:80:TRP:CE2	2.41	0.55
4:Q:134:TYR:CG	4:Q:162:PRO:HG3	2.41	0.55
2:O:192:HIS:O	2:O:196:GLN:HG3	2.06	0.55
2:O:403:ASP:O	2:O:405:VAL:N	2.38	0.55
3:C:286:PRO:O	3:C:287:ASN:CB	2.55	0.55
1:A:15:ASN:O	1:A:26:ALA:HA	2.04	0.55
8:U:65:ARG:O	8:U:68:CYS:HB3	2.06	0.55
3:C:9:HIS:CD2	3:C:11:LEU:H	2.24	0.55
13:P:3002:UQ:HM51	13:P:3002:UQ:C8	2.37	0.55
1:N:134:ILE:CG2	1:N:174:ILE:HD13	2.36	0.55
3:C:69:HIS:CD2	3:C:73:ASN:HD22	2.24	0.55
2:B:27:THR:CG2	2:B:28:LYS:N	2.70	0.55
8:H:17:LEU:HD13	8:H:73:LEU:HD22	1.87	0.55
1:N:362:ARG:O	1:N:365:MET:HG2	2.07	0.55
4:Q:222:MET:HE3	5:R:40:THR:HG23	1.89	0.55
1:A:402:VAL:HA	1:A:406:MET:HE1	1.89	0.55
1:N:140:GLU:OE2	9:V:50:LEU:N	2.37	0.55
2:B:345:LYS:HG2	2:B:418:VAL:CG1	2.36	0.55
2:O:46:ARG:HD2	2:O:110:GLU:HG2	1.89	0.55
1:A:90:THR:HB	1:A:95:THR:HG23	1.88	0.55
3:C:212:ILE:CD1	6:F:62:ILE:HG23	2.37	0.55
5:E:76:ILE:O	5:E:193:VAL:HG12	2.07	0.55
3:P:138:GLN:HB2	3:P:255:GLU:O	2.06	0.55
3:P:245:LEU:O	4:Q:201:ARG:CD	2.55	0.55
2:B:80:ALA:HA	2:B:84:ARG:NH1	2.21	0.55
9:V:34:UNK:N	9:V:35:UNK:N	2.54	0.55
2:O:47:ILE:HD11	2:O:116:VAL:CG1	2.35	0.55
4:Q:218:LEU:HD11	5:R:42:THR:CG2	2.37	0.55
2:B:52:LYS:O	2:B:203:ARG:NH2	2.40	0.55
5:E:75:GLU:HB3	5:E:194:VAL:HG22	1.88	0.55
3:P:34:PHE:HB2	20:P:381:HOH:O	2.06	0.55
3:P:136:TRP:HH2	3:P:171:VAL:HG12	1.71	0.55
3:P:101:ARG:C	3:P:101:ARG:HD2	2.28	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:357:VAL:CG1	2:O:361:LYS:HE3	2.35	0.54
2:O:57:TYR:N	2:O:57:TYR:CD1	2.74	0.54
1:N:373:THR:N	1:N:374:PRO:HD2	2.22	0.54
4:Q:74:PRO:HB2	4:Q:78:GLY:HA2	1.88	0.54
2:O:290:SER:O	2:O:297:GLN:HG2	2.07	0.54
1:N:196:VAL:HG11	1:N:383:LEU:HD12	1.89	0.54
4:Q:161:ALA:O	4:Q:162:PRO:C	2.45	0.54
4:D:74:PRO:HB2	4:D:78:GLY:HA2	1.89	0.54
4:Q:220:TYR:CZ	4:Q:224:ARG:HD3	2.42	0.54
9:V:69:SER:HB2	9:V:72:ALA:HB3	1.89	0.54
2:B:47:ILE:HG22	2:B:48:GLY:N	2.23	0.54
6:S:17:ARG:HG2	6:S:17:ARG:HH11	1.72	0.54
3:C:136:TRP:HH2	3:C:171:VAL:HG12	1.72	0.54
1:A:294:LEU:HD23	1:A:307:PHE:CZ	2.43	0.54
4:Q:139:ALA:HB2	8:U:41:ASP:OD1	2.07	0.54
3:P:9:HIS:CD2	3:P:11:LEU:H	2.25	0.54
3:P:112:GLU:O	3:P:116:THR:HG23	2.08	0.54
1:A:170:THR:HG22	1:A:171:THR:N	2.23	0.54
4:Q:237:TYR:HB2	6:S:60:PHE:CG	2.42	0.54
3:C:169:PHE:CE1	5:R:72:SER:HA	2.39	0.54
1:A:151:ASP:OD2	5:E:2:HIS:NE2	2.34	0.54
2:O:206:LEU:HD23	2:O:220:ALA:HB2	1.89	0.54
4:Q:117:VAL:HG21	4:Q:191:ARG:HA	1.90	0.54
3:C:22:LEU:HD21	13:C:2002:UQ:HM32	1.89	0.54
1:N:35:CYS:SG	1:N:203:ILE:HD11	2.48	0.54
1:N:85:HIS:NE2	2:O:284:LEU:HD22	2.23	0.54
2:O:100:SER:HB2	2:O:105:MET:HG2	1.90	0.54
3:C:245:LEU:O	4:D:201:ARG:CD	2.55	0.54
3:P:173:ASN:N	3:P:174:PRO:HD2	2.22	0.54
2:O:385:GLU:O	2:O:387:LEU:N	2.41	0.54
1:N:295:ALA:O	1:N:298:ALA:HB3	2.07	0.54
3:C:207:ASN:ND2	3:C:208:ASN:H	2.05	0.54
2:O:407:SER:O	2:O:411:VAL:HG23	2.08	0.54
4:D:8:PRO:HG2	4:D:10:PHE:CE1	2.42	0.54
2:O:307:PHE:CD1	2:O:308:ASP:N	2.76	0.54
3:C:142:TRP:O	3:C:146:VAL:HG23	2.07	0.54
6:S:73:ARG:NH1	7:T:32:ASP:OD2	2.41	0.54
4:Q:47:ALA:N	4:Q:50:ASN:HD22	1.91	0.54
1:A:255:LEU:HD12	1:A:422:LEU:HB2	1.90	0.54
8:U:73:LEU:HD12	8:U:73:LEU:O	2.08	0.54
3:P:69:HIS:CD2	3:P:73:ASN:HD22	2.26	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:ARG:NH2	1:A:177:LEU:O	2.41	0.54
3:P:329:LEU:O	3:P:332:ASN:HB3	2.08	0.54
2:B:402:ILE:HG23	2:B:403:ASP:N	2.23	0.54
5:R:135:LEU:HD23	5:R:182:VAL:HG22	1.91	0.54
5:R:76:ILE:O	5:R:193:VAL:HG12	2.08	0.54
2:B:57:TYR:HE2	2:B:203:ARG:HH22	1.45	0.54
1:N:209:VAL:O	1:N:212:ALA:HB3	2.08	0.54
4:D:12:TRP:CZ2	4:D:124:GLU:HB2	2.43	0.54
1:N:178:THR:HG22	1:N:180:ALA:N	2.09	0.53
2:B:318:ASP:O	2:B:319:SER:HB2	2.08	0.53
1:A:336:PHE:CZ	3:C:4:ASN:HB3	2.43	0.53
3:P:172:ASP:HB3	3:P:174:PRO:HD2	1.90	0.53
2:B:207:VAL:HG21	2:B:383:GLY:CA	2.38	0.53
6:S:91:GLU:HB3	6:S:92:PRO:HD3	1.91	0.53
4:D:47:ALA:H	4:D:50:ASN:ND2	1.96	0.53
2:O:46:ARG:HG3	2:O:379:LEU:HD22	1.90	0.53
13:C:2002:UQ:HM51	13:C:2002:UQ:C8	2.38	0.53
5:E:116:LYS:HD2	5:E:116:LYS:N	2.23	0.53
2:O:57:TYR:HE2	2:O:203:ARG:HH22	1.48	0.53
3:C:377:MET:HE2	6:F:20:TYR:CD1	2.43	0.53
2:B:168:TYR:CE2	2:B:172:LEU:HD12	2.43	0.53
1:A:182:LEU:O	1:A:186:ILE:HG13	2.07	0.53
2:B:96:LEU:H	9:I:70:LEU:HD22	1.74	0.53
1:A:282:ARG:NH2	9:I:35:UNK:HA	2.23	0.53
2:B:345:LYS:HG2	2:B:418:VAL:HG13	1.91	0.53
2:B:34:ILE:HD13	2:B:390:GLY:HA2	1.90	0.53
1:A:106:MET:HG3	1:A:203:ILE:CD1	2.34	0.53
2:B:47:ILE:HG21	2:B:120:MET:HE1	1.90	0.53
1:N:336:PHE:CZ	3:P:4:ASN:HB3	2.44	0.53
9:V:69:SER:CB	9:V:72:ALA:HB3	2.39	0.53
1:A:395:TRP:CE3	1:A:395:TRP:HA	2.43	0.53
5:E:117:LEU:HD23	5:E:121:GLN:H	1.73	0.53
5:R:112:VAL:HG21	5:R:170:ARG:NH2	2.24	0.53
2:B:28:LYS:O	2:B:29:LEU:O	2.27	0.53
1:A:136:GLN:OE1	9:I:50:LEU:HD12	2.08	0.53
5:E:86:ASN:ND2	5:E:148:ALA:HB2	2.22	0.53
9:V:28:UNK:CB	9:V:72:ALA:HB2	2.39	0.53
10:J:60:GLU:O	10:J:61:ALA:HB3	2.09	0.53
7:T:49:ALA:HB3	7:T:50:PRO:HD3	1.90	0.53
2:O:71:LEU:HD23	9:V:68:ILE:HG13	1.91	0.53
1:A:165:ARG:HG3	1:A:165:ARG:HH11	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:56:ARG:NH1	2:O:172:LEU:HG	2.24	0.53
3:C:92:PHE:O	3:C:95:ILE:HG22	2.08	0.53
2:B:99:TYR:HE1	2:B:108:CYS:SG	2.32	0.53
3:P:143:GLY:O	3:P:147:ILE:HG12	2.09	0.53
2:B:268:GLU:O	2:B:271:ALA:HB3	2.09	0.53
2:O:424:MET:HG2	2:O:425:ALA:N	2.24	0.53
1:N:191:LYS:CA	1:N:195:MET:HE2	2.39	0.53
3:P:156:TYR:CD2	3:P:156:TYR:N	2.75	0.53
6:F:94:LEU:O	6:F:94:LEU:HD12	2.08	0.53
2:O:109:VAL:HG21	2:O:119:VAL:HG12	1.91	0.52
2:B:357:VAL:O	2:B:361:LYS:HG3	2.09	0.52
5:R:134:ILE:HD12	5:R:185:TYR:CE1	2.43	0.52
1:N:9:GLN:HG2	1:N:393:GLU:OE2	2.10	0.52
2:O:132:PHE:CE1	2:O:191:LEU:HB3	2.44	0.52
2:O:140:LEU:C	2:O:142:PRO:HD2	2.28	0.52
2:O:207:VAL:HG21	2:O:383:GLY:CA	2.39	0.52
1:A:438:ARG:HH11	1:A:438:ARG:HG3	1.74	0.52
5:R:136:VAL:O	5:R:138:VAL:N	2.38	0.52
3:C:121:LEU:O	3:C:125:MET:HG3	2.08	0.52
10:W:59:TYR:N	10:W:59:TYR:CD1	2.76	0.52
2:B:140:LEU:C	2:B:142:PRO:HD2	2.30	0.52
5:E:117:LEU:HD23	5:E:119:ASP:O	2.10	0.52
3:P:92:PHE:O	3:P:95:ILE:HG22	2.08	0.52
3:P:305:ILE:HB	3:P:306:PRO:HD3	1.91	0.52
2:O:124:LEU:HD11	2:O:223:PHE:HB3	1.92	0.52
1:A:64:PHE:HE2	1:A:86:PHE:CE1	2.28	0.52
3:C:305:ILE:HB	3:C:306:PRO:HD3	1.92	0.52
3:P:49:GLY:C	12:P:501:HEM:HAC	2.30	0.52
2:O:56:ARG:HH12	2:O:172:LEU:HG	1.74	0.52
4:Q:229:VAL:HG23	7:T:20:PRO:HG3	1.92	0.52
3:P:347:PRO:O	3:P:351:ILE:HG13	2.09	0.52
3:P:278:ALA:HB1	3:P:295:LEU:HD12	1.91	0.52
3:C:99:ILE:HD11	3:C:121:LEU:HD22	1.91	0.52
2:O:67:HIS:O	2:O:70:ARG:HB3	2.10	0.52
2:O:325:TYR:CD1	9:V:60:ALA:HB3	2.45	0.52
4:D:220:TYR:CZ	4:D:224:ARG:HD3	2.44	0.52
6:S:42:ASP:OD1	6:S:101:ARG:NH1	2.43	0.52
1:N:39:VAL:HA	1:N:196:VAL:O	2.10	0.52
3:C:215:ASP:HA	3:C:218:LYS:HE2	1.90	0.52
4:D:68:VAL:HG12	4:D:69:GLU:N	2.24	0.52
1:A:359:ASN:HD22	2:B:92:VAL:HA	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:101:ARG:C	3:C:101:ARG:HD2	2.30	0.52
2:B:170:THR:O	2:B:172:LEU:N	2.43	0.52
3:P:202:HIS:NE2	13:P:3002:UQ:O4	2.38	0.52
1:A:191:LYS:N	1:A:195:MET:HE2	2.25	0.52
2:O:130:PRO:HB2	2:O:132:PHE:CE2	2.45	0.52
7:G:36:ASN:O	7:G:40:ARG:HG3	2.10	0.52
4:D:161:ALA:O	4:D:162:PRO:C	2.48	0.52
5:R:171:ILE:HD13	5:R:176:ALA:HB3	1.92	0.52
2:B:57:TYR:CD1	2:B:57:TYR:N	2.77	0.52
1:N:137:GLU:O	1:N:141:MET:HG3	2.09	0.52
6:F:32:MET:O	6:F:33:ARG:C	2.49	0.52
4:Q:12:TRP:CZ2	4:Q:124:GLU:HB2	2.44	0.52
1:A:362:ARG:O	1:A:365:MET:HG2	2.09	0.52
6:F:67:ASP:CG	6:F:71:LYS:HZ3	2.12	0.52
3:C:342:GLN:HB3	3:C:343:PRO:HD2	1.92	0.52
2:O:212:LYS:HB3	2:O:215:ASP:OD2	2.09	0.52
2:B:338:ARG:O	2:B:341:MET:HB2	2.10	0.51
2:O:341:MET:HA	2:O:341:MET:CE	2.40	0.51
3:C:319:ARG:HD2	3:C:374:GLU:OE2	2.10	0.51
2:O:34:ILE:HD13	2:O:390:GLY:HA2	1.92	0.51
5:R:81:ILE:HG12	5:R:87:VAL:HG21	1.91	0.51
8:U:40:CYS:O	8:U:44:VAL:HG23	2.10	0.51
1:A:404:ALA:O	1:A:406:MET:N	2.43	0.51
3:P:282:LEU:HD12	3:P:291:GLY:O	2.10	0.51
2:O:56:ARG:HG3	2:O:56:ARG:NH1	2.25	0.51
2:B:63:LEU:HB2	2:B:182:ARG:CD	2.38	0.51
1:A:307:PHE:C	1:A:307:PHE:CD1	2.83	0.51
3:C:23:PRO:HG2	7:G:3:HIS:HB3	1.93	0.51
2:B:262:ALA:O	2:B:320:GLY:HA3	2.11	0.51
3:P:377:MET:HE2	6:S:20:TYR:CG	2.45	0.51
2:B:35:ILE:HD13	2:B:217:LYS:HA	1.92	0.51
2:O:38:LEU:HD12	2:O:38:LEU:C	2.31	0.51
2:B:22:GLU:HG3	2:B:23:ASP:H	1.74	0.51
5:E:190:ASP:O	5:E:192:LEU:N	2.43	0.51
2:O:414:ALA:O	2:O:418:VAL:HG23	2.11	0.51
2:O:156:GLN:HE22	9:V:77:ARG:C	2.14	0.51
2:O:341:MET:HA	2:O:341:MET:HE2	1.92	0.51
2:O:170:THR:O	2:O:172:LEU:N	2.43	0.51
2:O:318:ASP:O	2:O:319:SER:HB2	2.11	0.51
4:D:167:GLU:HG3	8:H:13:LEU:HD23	1.91	0.51
4:D:102:ARG:HA	4:D:108:ALA:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:65:ARG:O	8:H:68:CYS:HB3	2.10	0.51
5:E:52:LYS:C	5:E:52:LYS:HD3	2.30	0.51
1:N:10:ASN:ND2	2:O:19:PRO:HD2	2.26	0.51
1:N:178:THR:CG2	1:N:179:ARG:N	2.73	0.51
2:O:46:ARG:HG3	2:O:46:ARG:O	2.10	0.51
2:B:38:LEU:HD12	2:B:39:GLU:N	2.26	0.51
2:B:80:ALA:HA	2:B:84:ARG:HH12	1.75	0.51
2:B:307:PHE:CD1	2:B:308:ASP:N	2.79	0.51
2:B:407:SER:O	2:B:411:VAL:HG23	2.11	0.51
3:C:173:ASN:N	3:C:174:PRO:HD2	2.26	0.51
10:J:58:LYS:HB2	10:J:59:TYR:CE1	2.45	0.51
7:T:24:ARG:HB2	7:T:27:PRO:HB3	1.93	0.51
8:H:40:CYS:O	8:H:44:VAL:HG23	2.10	0.51
1:N:106:MET:HE2	1:N:106:MET:O	2.10	0.51
5:R:103:GLN:HA	5:R:106:ILE:HD12	1.93	0.51
5:R:96:LEU:HD21	5:R:195:VAL:HG21	1.92	0.51
1:N:295:ALA:O	1:N:299:VAL:HG23	2.10	0.51
1:N:321:GLY:HA2	1:N:342:TRP:CZ2	2.42	0.51
5:E:135:LEU:CD1	5:E:169:GLY:HA3	2.40	0.51
4:Q:151:PRO:HA	4:Q:156:GLN:HG3	1.92	0.51
14:P:3004:CDL:HA32	7:T:40:ARG:HB3	1.92	0.51
3:P:31:TRP:CZ3	15:P:3007:PEE:H20	2.46	0.51
2:B:56:ARG:NH1	2:B:172:LEU:HG	2.26	0.51
1:A:321:GLY:HA2	1:A:342:TRP:CZ2	2.45	0.51
3:P:332:ASN:ND2	3:P:358:SER:OG	2.42	0.51
1:A:117:VAL:HG23	1:A:118:GLN:HG3	1.93	0.51
3:C:246:PHE:C	3:C:248:PRO:HD3	2.31	0.51
4:Q:47:ALA:O	4:Q:50:ASN:HB2	2.11	0.50
5:E:130:PRO:C	5:E:132:TRP:H	2.14	0.50
1:N:64:PHE:HE2	1:N:86:PHE:CE1	2.30	0.50
2:O:247:GLN:HE22	2:O:429:ASP:HA	1.75	0.50
1:A:121:ALA:O	1:A:122:LEU:HB2	2.11	0.50
5:E:130:PRO:HG2	5:E:131:GLU:CD	2.32	0.50
3:C:138:GLN:HB2	3:C:255:GLU:O	2.11	0.50
1:N:26:ALA:O	1:N:198:ALA:HA	2.12	0.50
5:E:129:LYS:HG3	5:E:187:PHE:CZ	2.46	0.50
2:B:273:SER:O	2:B:276:GLN:HB3	2.11	0.50
4:D:168:ILE:HG12	4:D:168:ILE:O	2.10	0.50
7:G:50:PRO:HB2	7:G:51:PRO:HD3	1.92	0.50
2:O:402:ILE:HG23	2:O:403:ASP:N	2.26	0.50
2:O:395:PRO:HA	2:O:398:VAL:HG12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:LEU:HD22	1:A:320:PHE:CE1	2.46	0.50
3:C:327:TRP:CE2	7:G:48:VAL:HG22	2.46	0.50
1:A:134:ILE:HG21	1:A:174:ILE:HD13	1.94	0.50
1:N:395:TRP:HA	1:N:395:TRP:HE3	1.76	0.50
5:R:162:GLY:O	5:R:163:SER:C	2.50	0.50
5:R:81:ILE:HD13	5:R:98:VAL:O	2.11	0.50
1:N:255:LEU:CD1	1:N:422:LEU:HB2	2.40	0.50
3:P:105:TYR:CA	3:P:315:THR:HG22	2.41	0.50
2:B:141:GLN:N	2:B:142:PRO:HD2	2.27	0.50
6:F:53:ASP:OD1	6:F:54:LEU:N	2.44	0.50
3:P:48:THR:HG1	3:P:84:HIS:HD1	1.57	0.50
9:V:64:LEU:HD12	9:V:77:ARG:O	2.12	0.50
1:A:37:VAL:HG23	1:A:113:LEU:HD11	1.94	0.50
2:O:341:MET:HE1	2:O:417:PHE:CE2	2.34	0.50
1:N:255:LEU:O	1:N:321:GLY:HA3	2.12	0.50
3:C:105:TYR:CA	3:C:315:THR:HG22	2.41	0.50
2:B:414:ALA:O	2:B:418:VAL:HG23	2.12	0.50
4:Q:183:ALA:O	4:Q:186:VAL:HG12	2.12	0.50
7:T:50:PRO:HB2	7:T:51:PRO:HD3	1.91	0.50
2:O:141:GLN:N	2:O:142:PRO:HD2	2.26	0.50
4:D:102:ARG:HG2	4:D:102:ARG:HH11	1.75	0.50
1:A:196:VAL:HG11	1:A:383:LEU:HD12	1.93	0.50
1:A:343:MET:HB3	1:A:444:ILE:HA	1.94	0.50
2:B:341:MET:HA	2:B:341:MET:CE	2.42	0.50
5:E:72:SER:HA	3:P:169:PHE:CE1	2.46	0.50
7:G:36:ASN:OD1	7:G:39:ARG:NH1	2.42	0.50
10:J:59:TYR:CD1	10:J:59:TYR:N	2.79	0.50
4:Q:102:ARG:HA	4:Q:108:ALA:O	2.12	0.50
3:C:31:TRP:NE1	15:C:2007:PEE:O4	2.45	0.50
3:P:327:TRP:CE2	7:T:48:VAL:HG22	2.47	0.50
3:C:347:PRO:O	3:C:351:ILE:HG13	2.12	0.50
5:R:171:ILE:CD1	5:R:176:ALA:HB3	2.41	0.50
1:N:117:VAL:HG23	1:N:118:GLN:HG3	1.93	0.50
1:N:317:THR:HG23	1:N:318:GLY:N	2.27	0.50
7:G:72:LYS:HE2	8:H:57:GLU:OE1	2.12	0.50
17:Q:501:HEC:HMB1	17:Q:501:HEC:HBB3	1.94	0.50
2:O:18:CYS:HB3	2:O:19:PRO:HD2	1.94	0.49
1:A:106:MET:O	1:A:110:VAL:HG23	2.11	0.49
3:P:18:SER:HB2	3:P:202:HIS:HE1	1.77	0.49
1:A:255:LEU:O	1:A:321:GLY:HA3	2.11	0.49
3:C:28:ILE:HD11	3:C:225:TYR:CZ	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:183:ALA:O	4:D:186:VAL:HG12	2.11	0.49
1:N:178:THR:HB	1:N:181:ASP:OD1	2.12	0.49
2:B:109:VAL:HG21	2:B:119:VAL:HG12	1.94	0.49
2:B:46:ARG:HG3	2:B:46:ARG:O	2.11	0.49
1:N:186:ILE:HG23	1:N:190:PHE:CD1	2.47	0.49
4:Q:220:TYR:O	4:Q:224:ARG:HG2	2.12	0.49
4:Q:215:LEU:HD13	5:R:46:ALA:HB3	1.94	0.49
6:F:73:ARG:NH1	7:G:32:ASP:OD2	2.45	0.49
5:E:84:GLY:N	5:E:100:HIS:O	2.43	0.49
1:N:281:ASP:HB3	1:N:284:PHE:CE1	2.46	0.49
2:O:206:LEU:O	2:O:206:LEU:HG	2.12	0.49
1:A:186:ILE:HG23	1:A:190:PHE:CD1	2.46	0.49
2:B:353:THR:HG22	2:B:355:GLU:N	2.10	0.49
5:E:84:GLY:CA	5:E:102:THR:HG23	2.42	0.49
9:I:70:LEU:HG	9:I:71:ASN:N	2.26	0.49
1:A:63:ALA:O	1:A:116:VAL:HG13	2.12	0.49
2:O:80:ALA:HA	2:O:84:ARG:NH1	2.27	0.49
5:R:52:LYS:HD3	5:R:52:LYS:C	2.33	0.49
3:P:45:GLN:CB	12:P:501:HEM:HAB	2.43	0.49
4:D:229:VAL:CG2	7:G:20:PRO:HG3	2.43	0.49
3:P:27:ASN:ND2	3:P:209:PRO:HG2	2.27	0.49
1:A:39:VAL:HG11	1:A:117:VAL:HG11	1.95	0.49
3:C:31:TRP:CZ3	15:C:2007:PEE:H20	2.48	0.49
3:P:247:SER:OG	3:P:250:LEU:HB2	2.13	0.49
2:B:280:GLY:HA3	2:B:293:SER:OG	2.12	0.49
6:S:71:LYS:O	6:S:72:HIS:HB2	2.13	0.49
3:C:238:THR:HB	3:C:239:PRO:CD	2.36	0.49
5:E:127:VAL:O	5:E:128:LYS:HB2	2.13	0.49
2:O:56:ARG:NH1	2:O:171:ALA:HB1	2.27	0.49
1:A:49:ASN:HD21	1:A:51:LYS:H	1.59	0.49
3:P:9:HIS:CD2	3:P:11:LEU:HB2	2.48	0.49
3:P:105:TYR:CD2	3:P:209:PRO:HA	2.48	0.49
1:N:165:ARG:HG3	1:N:165:ARG:NH1	2.26	0.49
1:A:26:ALA:O	1:A:198:ALA:HA	2.13	0.49
2:B:207:VAL:HG21	2:B:383:GLY:HA3	1.95	0.49
1:N:433:ASP:OD2	1:N:435:ASN:HB2	2.12	0.49
4:Q:227:TRP:O	4:Q:228:SER:C	2.51	0.49
2:B:248:ASN:ND2	2:B:248:ASN:C	2.64	0.49
1:N:173:ASN:O	1:N:177:LEU:HG	2.13	0.49
14:P:3004:CDL:OA4	7:T:40:ARG:HD2	2.13	0.49
3:P:319:ARG:O	3:P:323:GLN:HG3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:56:ARG:HG3	2:B:56:ARG:NH1	2.24	0.49
1:A:206:LYS:HA	1:A:209:VAL:CG1	2.42	0.49
14:D:2003:CDL:H721	14:D:2003:CDL:HA62	1.93	0.49
3:C:112:GLU:O	3:C:116:THR:HG23	2.12	0.49
3:P:333:LEU:HD21	3:P:359:TYR:CE1	2.48	0.49
5:R:137:GLY:O	5:R:145:VAL:HG13	2.12	0.49
2:B:56:ARG:HH12	2:B:172:LEU:HG	1.76	0.49
3:C:49:GLY:C	12:C:501:HEM:HAC	2.33	0.49
2:B:200:THR:OG1	2:B:203:ARG:HG3	2.13	0.49
1:A:23:LEU:C	1:A:23:LEU:HD23	2.33	0.49
9:V:32:UNK:O	9:V:33:UNK:C	2.61	0.49
7:T:36:ASN:OD1	7:T:39:ARG:NH1	2.45	0.49
2:O:129:ALA:N	2:O:130:PRO:CD	2.76	0.49
4:D:37:CYS:O	4:D:39:ALA:N	2.44	0.49
1:N:121:ALA:O	1:N:122:LEU:HB2	2.12	0.49
2:O:96:LEU:HD12	2:O:97:SER:N	2.28	0.49
2:O:168:TYR:CE2	2:O:172:LEU:HD12	2.48	0.49
3:P:292:VAL:O	3:P:295:LEU:HB3	2.13	0.49
1:N:354:VAL:HG23	1:N:355:LYS:N	2.28	0.49
5:E:74:ILE:HG22	5:E:91:TRP:CD1	2.48	0.49
3:P:246:PHE:C	3:P:248:PRO:HD3	2.33	0.49
5:R:119:ASP:HB3	5:R:179:ASN:HD21	1.77	0.48
2:B:29:LEU:HB3	2:B:30:PRO:CD	2.43	0.48
1:A:85:HIS:HB2	1:A:100:LYS:HB2	1.94	0.48
2:O:39:GLU:OE2	2:O:113:ARG:NH2	2.46	0.48
14:Q:3003:CDL:HB22	7:T:40:ARG:NH2	2.27	0.48
9:V:51:CYS:HB2	9:V:53:GLU:OE1	2.13	0.48
6:F:77:LYS:HA	6:F:80:TRP:CE2	2.48	0.48
3:C:45:GLN:HB3	12:C:501:HEM:HAB	1.95	0.48
7:G:3:HIS:O	7:G:7:LEU:HG	2.12	0.48
14:D:2003:CDL:HB22	7:G:40:ARG:NH2	2.28	0.48
1:A:279:ARG:HH22	9:I:30:UNK:C	2.26	0.48
9:V:49:LEU:HD13	9:V:55:MET:HG2	1.94	0.48
1:N:307:PHE:CD1	1:N:307:PHE:C	2.85	0.48
5:E:171:ILE:HG22	5:E:179:ASN:OD1	2.12	0.48
3:P:286:PRO:O	3:P:287:ASN:CB	2.61	0.48
4:Q:150:ASN:O	4:Q:156:GLN:HA	2.13	0.48
3:P:6:ARG:HG2	3:P:16:ASN:HB2	1.95	0.48
9:V:70:LEU:HD23	9:V:71:ASN:H	1.78	0.48
3:P:342:GLN:HB3	3:P:343:PRO:HD2	1.95	0.48
4:D:195:GLU:OE1	4:D:201:ARG:NH2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:158:ILE:HG12	4:Q:160:MET:H	1.78	0.48
1:N:361:LEU:O	1:N:364:ALA:HB3	2.14	0.48
4:D:47:ALA:HA	4:D:90:TYR:HA	1.95	0.48
2:B:129:ALA:N	2:B:130:PRO:CD	2.77	0.48
2:B:247:GLN:HE22	2:B:429:ASP:HA	1.78	0.48
1:A:178:THR:CG2	1:A:179:ARG:N	2.76	0.48
4:Q:178:THR:CG2	8:U:15:ASP:HA	2.43	0.48
3:C:319:ARG:O	3:C:323:GLN:HG3	2.13	0.48
5:E:163:SER:HA	5:E:174:GLY:HA3	1.95	0.48
2:B:312:PHE:HE1	9:I:62:ARG:O	1.96	0.48
2:B:295:LEU:O	2:B:299:VAL:HG23	2.14	0.48
3:P:28:ILE:HD11	3:P:225:TYR:CZ	2.48	0.48
2:O:374:THR:HG22	2:O:376:GLN:H	1.79	0.48
1:A:295:ALA:O	1:A:299:VAL:HG23	2.14	0.48
4:Q:116:ILE:CG2	4:Q:190:LEU:HD13	2.43	0.48
1:N:191:LYS:C	1:N:193:PRO:HD2	2.34	0.48
1:A:39:VAL:HA	1:A:196:VAL:O	2.13	0.48
1:A:344:ARG:HH22	1:A:353:GLU:CD	2.16	0.48
2:O:221:GLU:HG3	2:O:222:GLN:N	2.21	0.48
5:E:102:THR:C	5:E:103:GLN:HG3	2.34	0.48
2:O:248:ASN:C	2:O:248:ASN:ND2	2.64	0.48
1:N:280:TYR:CG	1:N:281:ASP:N	2.81	0.48
3:C:233:LEU:O	3:C:237:LEU:HB2	2.12	0.48
3:P:319:ARG:HD2	3:P:374:GLU:OE2	2.14	0.48
4:D:150:ASN:O	4:D:156:GLN:HA	2.13	0.48
10:W:57:HIS:ND1	10:W:58:LYS:N	2.62	0.48
5:R:95:PRO:HG2	5:R:145:VAL:HG11	1.95	0.48
4:D:37:CYS:C	4:D:39:ALA:N	2.67	0.48
4:D:117:VAL:HG21	4:D:191:ARG:HA	1.96	0.48
4:Q:68:VAL:HG11	4:Q:92:PRO:CG	2.44	0.48
3:C:198:LEU:HD21	12:C:502:HEM:CMA	2.44	0.48
4:D:227:TRP:O	4:D:228:SER:C	2.51	0.48
1:N:170:THR:HG22	1:N:171:THR:H	1.78	0.48
2:O:353:THR:HG22	2:O:355:GLU:N	2.09	0.47
1:N:402:VAL:HA	1:N:406:MET:HE1	1.96	0.47
3:P:377:MET:HE2	6:S:20:TYR:CD1	2.49	0.47
4:D:37:CYS:C	4:D:39:ALA:H	2.16	0.47
4:Q:235:MET:HB3	7:T:15:THR:HG22	1.96	0.47
9:I:55:MET:O	9:I:58:ARG:HG2	2.13	0.47
3:C:6:ARG:HG2	3:C:16:ASN:HB2	1.95	0.47
2:O:35:ILE:HD13	2:O:217:LYS:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:403:ASP:O	2:B:405:VAL:N	2.44	0.47
3:P:146:VAL:HG21	3:P:269:ILE:HG21	1.95	0.47
2:B:385:GLU:C	2:B:387:LEU:H	2.17	0.47
14:C:2004:CDL:OA4	7:G:40:ARG:HD2	2.14	0.47
5:E:35:PHE:O	5:E:38:LEU:HB3	2.15	0.47
2:B:259:THR:HG22	2:B:260:GLU:N	2.30	0.47
5:E:119:ASP:O	5:E:121:GLN:N	2.47	0.47
7:T:3:HIS:O	7:T:7:LEU:HG	2.13	0.47
9:I:49:LEU:O	9:I:50:LEU:HD23	2.15	0.47
1:A:240:GLU:HA	1:A:422:LEU:O	2.14	0.47
4:D:134:TYR:CE1	4:D:162:PRO:HA	2.49	0.47
7:T:68:ARG:NH2	7:T:69:LEU:HD21	2.29	0.47
5:E:165:TYR:HA	5:E:170:ARG:O	2.15	0.47
2:O:47:ILE:CD1	2:O:116:VAL:HG13	2.39	0.47
2:B:374:THR:HG22	2:B:376:GLN:H	1.79	0.47
2:O:38:LEU:HD12	2:O:39:GLU:N	2.29	0.47
2:B:306:PRO:HA	9:I:52:ARG:CG	2.45	0.47
5:R:83:GLU:HB3	5:R:102:THR:HG22	1.95	0.47
9:I:70:LEU:CD2	9:I:71:ASN:N	2.78	0.47
1:N:23:LEU:HD23	1:N:23:LEU:C	2.35	0.47
1:A:170:THR:HB	1:A:173:ASN:HB2	1.96	0.47
1:N:79:VAL:O	1:N:82:MET:HG2	2.14	0.47
3:C:36:SER:O	3:C:40:VAL:HG23	2.14	0.47
5:E:188:VAL:HG12	5:E:188:VAL:O	2.14	0.47
1:N:438:ARG:HH11	1:N:438:ARG:HG3	1.80	0.47
5:R:144:CYS:HB2	5:R:158:CYS:SG	2.54	0.47
9:V:70:LEU:HD23	9:V:71:ASN:N	2.30	0.47
1:A:134:ILE:CG2	1:A:174:ILE:HD13	2.45	0.47
1:A:395:TRP:HA	1:A:395:TRP:HE3	1.78	0.47
4:D:116:ILE:CG2	4:D:190:LEU:HD13	2.43	0.47
5:R:96:LEU:HD12	5:R:135:LEU:O	2.14	0.47
5:R:153:PHE:O	5:R:155:GLY:N	2.48	0.47
3:P:92:PHE:O	3:P:93:ILE:C	2.52	0.47
3:C:92:PHE:O	3:C:93:ILE:C	2.50	0.47
3:P:105:TYR:CE2	3:P:209:PRO:HA	2.50	0.47
7:T:36:ASN:O	7:T:40:ARG:HG3	2.14	0.47
4:D:122:GLY:O	4:D:123:GLY:C	2.53	0.47
2:B:102:ARG:NE	2:B:164:HIS:CD2	2.82	0.47
1:N:289:HIS:CD2	2:O:83:PHE:HD1	2.32	0.47
7:G:68:ARG:NH2	7:G:69:LEU:HD21	2.29	0.47
2:B:206:LEU:O	2:B:216:LEU:HD21	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:46:ARG:NH1	1:N:93:GLU:OE2	2.47	0.47
5:E:10:PHE:CD1	7:G:18:LEU:HD21	2.50	0.47
10:W:20:PHE:O	10:W:24:VAL:HG23	2.15	0.47
1:A:106:MET:O	1:A:106:MET:HE2	2.15	0.47
3:P:106:GLY:HA2	3:P:108:TYR:CZ	2.50	0.47
4:Q:139:ALA:HB1	8:U:44:VAL:HB	1.96	0.47
3:P:44:THR:O	3:P:48:THR:HG23	2.15	0.47
5:R:79:SER:OG	5:R:191:ASP:HB2	2.15	0.47
2:B:292:THR:O	2:B:292:THR:HG22	2.15	0.47
1:N:219:VAL:HG12	1:N:220:SER:N	2.30	0.47
4:D:47:ALA:O	4:D:50:ASN:HB2	2.14	0.47
1:N:49:ASN:HD21	1:N:51:LYS:H	1.57	0.47
3:P:18:SER:HA	3:P:22:LEU:HD22	1.96	0.47
1:N:253:VAL:O	1:N:323:HIS:HA	2.14	0.47
4:Q:134:TYR:CE1	4:Q:162:PRO:HA	2.50	0.47
3:C:22:LEU:HD12	3:C:23:PRO:N	2.29	0.47
1:N:47:TYR:CE2	1:N:231:LEU:HD11	2.49	0.47
2:O:31:ASN:N	2:O:31:ASN:HD22	2.13	0.47
2:O:31:ASN:ND2	2:O:31:ASN:N	2.63	0.47
1:N:10:ASN:HD21	2:O:19:PRO:HD2	1.79	0.46
3:C:292:VAL:O	3:C:295:LEU:HB3	2.15	0.46
2:B:28:LYS:HG2	2:B:28:LYS:O	2.14	0.46
1:N:85:HIS:HB2	1:N:100:LYS:HB2	1.97	0.46
2:O:345:LYS:HG2	2:O:418:VAL:HG11	1.97	0.46
3:P:141:PHE:HE1	3:P:171:VAL:O	1.97	0.46
4:D:220:TYR:O	4:D:224:ARG:HG2	2.15	0.46
5:E:140:THR:O	5:E:177:PRO:HD2	2.15	0.46
4:D:17:PRO:O	4:D:202:LYS:HD3	2.14	0.46
8:U:15:ASP:O	8:U:17:LEU:N	2.49	0.46
6:S:53:ASP:OD1	6:S:54:LEU:N	2.48	0.46
3:C:335:ILE:HD13	7:G:58:LEU:HD23	1.96	0.46
6:S:61:ARG:NH2	6:S:89:TYR:CE2	2.84	0.46
1:N:205:HIS:O	1:N:208:LEU:HB3	2.14	0.46
5:R:134:ILE:HD12	5:R:185:TYR:HD1	1.75	0.46
3:C:146:VAL:HG21	3:C:269:ILE:HG21	1.96	0.46
4:Q:102:ARG:HH11	4:Q:102:ARG:HG2	1.79	0.46
5:E:162:GLY:O	5:E:163:SER:C	2.53	0.46
2:O:33:LEU:HD12	2:O:204:MET:O	2.15	0.46
5:R:179:ASN:O	5:R:180:LEU:C	2.54	0.46
4:D:57:THR:HG22	4:D:58:GLU:N	2.30	0.46
2:O:207:VAL:HG21	2:O:383:GLY:HA3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:GLN:HG2	1:A:393:GLU:OE2	2.15	0.46
5:R:140:THR:OG1	5:R:176:ALA:HB1	2.16	0.46
5:R:163:SER:OG	5:R:176:ALA:HB2	2.16	0.46
3:P:278:ALA:HB1	3:P:295:LEU:HD11	1.96	0.46
1:A:255:LEU:CD1	1:A:422:LEU:HB2	2.46	0.46
2:B:424:MET:HG2	2:B:425:ALA:N	2.30	0.46
3:C:202:HIS:NE2	13:C:2002:UQ:O4	2.46	0.46
1:A:27:SER:HA	1:A:199:ALA:O	2.15	0.46
2:B:206:LEU:HG	2:B:206:LEU:O	2.15	0.46
8:H:15:ASP:O	8:H:17:LEU:N	2.48	0.46
4:D:239:PRO:HG2	4:D:241:LYS:HB2	1.97	0.46
2:B:370:MET:O	2:B:373:GLU:HG3	2.15	0.46
4:Q:168:ILE:HG12	4:Q:168:ILE:O	2.15	0.46
9:I:38:UNK:O	9:I:40:UNK:N	2.47	0.46
5:R:165:TYR:HA	5:R:170:ARG:O	2.15	0.46
3:C:9:HIS:CD2	3:C:11:LEU:HB2	2.51	0.46
5:E:141:HIS:HB3	19:E:501:FES:S2	2.55	0.46
1:A:289:HIS:CD2	2:B:83:PHE:HD1	2.32	0.46
2:B:366:ALA:O	2:B:369:LEU:N	2.49	0.46
5:E:131:GLU:H	5:E:131:GLU:CD	2.18	0.46
5:R:185:TYR:O	5:R:186:GLN:HB3	2.16	0.46
1:A:64:PHE:C	1:A:66:GLY:H	2.20	0.46
3:C:172:ASP:HB3	3:C:174:PRO:HD2	1.98	0.46
6:S:31:LEU:HD21	6:S:65:ALA:HB2	1.97	0.46
5:R:181:GLU:HG2	5:R:182:VAL:N	2.30	0.46
5:R:185:TYR:HB3	5:R:195:VAL:HA	1.98	0.46
8:U:44:VAL:HG21	8:U:54:CYS:SG	2.56	0.46
5:E:133:VAL:HG13	5:E:133:VAL:O	2.15	0.46
3:C:216:SER:HB3	6:F:59:MET:CE	2.46	0.46
2:O:33:LEU:CD2	2:O:224:LEU:HD12	2.46	0.46
2:O:307:PHE:HD1	2:O:308:ASP:N	2.14	0.46
2:O:133:ARG:HD3	2:O:135:TRP:CZ2	2.51	0.46
1:N:151:ASP:OD2	5:R:2:HIS:NE2	2.37	0.46
4:D:221:TYR:CD2	5:E:39:VAL:HG11	2.50	0.46
2:O:355:GLU:O	2:O:358:THR:N	2.49	0.45
1:A:35:CYS:SG	1:A:203:ILE:HD11	2.57	0.45
2:B:47:ILE:CD1	2:B:116:VAL:HG13	2.42	0.45
5:R:185:TYR:CD2	5:R:185:TYR:N	2.85	0.45
2:O:57:TYR:N	2:O:57:TYR:HD1	2.14	0.45
2:O:422:LYS:C	2:O:436:LEU:HD21	2.36	0.45
2:O:71:LEU:CD2	9:V:68:ILE:HG13	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:96:LEU:HD12	5:E:135:LEU:O	2.16	0.45
4:Q:181:GLN:HE21	4:Q:185:ASP:CG	2.19	0.45
2:O:385:GLU:C	2:O:387:LEU:H	2.19	0.45
2:B:135:TRP:O	2:B:136:GLU:C	2.53	0.45
5:E:144:CYS:HB2	5:E:158:CYS:SG	2.56	0.45
1:A:217:SER:O	1:A:218:GLY:C	2.54	0.45
7:T:79:ASN:O	7:T:80:ASP:HB2	2.16	0.45
2:O:198:ASN:O	2:O:203:ARG:HD3	2.16	0.45
5:E:52:LYS:NZ	10:J:32:GLU:OE1	2.42	0.45
2:O:327:ILE:HD11	9:V:58:ARG:O	2.16	0.45
4:D:29:GLY:HA3	4:D:189:PHE:HB2	1.98	0.45
1:A:48:GLU:HB3	1:A:52:ASN:OD1	2.16	0.45
1:N:34:THR:HA	1:N:102:LEU:HA	1.97	0.45
1:N:436:ARG:HA	1:N:436:ARG:HD2	1.77	0.45
6:F:67:ASP:HA	6:F:70:LEU:HD23	1.98	0.45
3:C:278:ALA:HB1	3:C:295:LEU:HD11	1.96	0.45
2:B:57:TYR:HE2	2:B:203:ARG:NH2	2.09	0.45
3:C:95:ILE:HD13	3:C:121:LEU:HD13	1.99	0.45
1:N:64:PHE:C	1:N:66:GLY:H	2.20	0.45
1:A:52:ASN:OD1	1:A:52:ASN:C	2.55	0.45
1:A:245:ASP:OD1	1:A:247:ALA:HB3	2.16	0.45
4:D:208:MET:C	4:D:208:MET:SD	2.95	0.45
7:G:34:LEU:HB2	7:G:35:PRO:HD3	1.98	0.45
8:H:28:GLU:O	8:H:32:LYS:HG3	2.16	0.45
3:C:273:TRP:CG	3:C:274:TYR:N	2.84	0.45
2:B:26:ILE:HG23	2:B:26:ILE:O	2.16	0.45
1:A:146:THR:O	1:A:150:PHE:HD1	1.98	0.45
4:D:57:THR:HG22	4:D:59:ALA:H	1.81	0.45
1:N:48:GLU:HB3	1:N:52:ASN:OD1	2.16	0.45
2:O:56:ARG:NH2	2:O:318:ASP:OD2	2.50	0.45
2:B:306:PRO:HB3	9:I:52:ARG:N	2.31	0.45
1:N:48:GLU:CD	1:N:54:GLY:H	2.20	0.45
9:V:38:UNK:O	9:V:39:UNK:CB	2.63	0.45
6:F:61:ARG:NH2	6:F:89:TYR:CE2	2.84	0.45
5:R:106:ILE:O	5:R:109:GLU:HB3	2.17	0.45
6:S:11:ARG:HA	6:S:14:ASP:HB2	1.98	0.45
8:H:10:GLU:O	8:H:11:GLU:HG3	2.17	0.45
4:Q:221:TYR:CD2	5:R:39:VAL:HG11	2.52	0.45
3:C:109:LEU:HD23	3:C:109:LEU:HA	1.84	0.45
3:P:238:THR:CB	3:P:239:PRO:HD3	2.34	0.45
5:E:86:ASN:OD1	5:E:99:ARG:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:376:LYS:O	6:S:17:ARG:NH1	2.50	0.45
1:A:264:ASP:HA	1:A:265:PRO:HD3	1.78	0.45
1:N:19:LEU:HB2	1:N:21:ASN:OD1	2.17	0.45
7:T:56:TYR:O	7:T:59:TYR:HB3	2.16	0.45
6:S:94:LEU:O	6:S:94:LEU:HD12	2.17	0.45
2:B:47:ILE:HD13	2:B:120:MET:SD	2.56	0.45
2:O:341:MET:CE	2:O:417:PHE:CE2	2.98	0.45
5:R:112:VAL:HG11	5:R:170:ARG:NH2	2.32	0.45
3:P:99:ILE:HD11	3:P:121:LEU:HD22	1.98	0.45
1:A:191:LYS:C	1:A:195:MET:HE2	2.37	0.45
3:C:28:ILE:CD1	13:C:2002:UQ:HM21	2.47	0.45
2:O:132:PHE:CD1	2:O:191:LEU:HB3	2.51	0.45
6:F:13:MET:O	6:F:17:ARG:HG3	2.15	0.45
2:B:110:GLU:O	2:B:111:CYS:HB3	2.17	0.45
3:C:287:ASN:O	3:C:288:LYS:C	2.55	0.45
5:R:133:VAL:HG13	5:R:133:VAL:O	2.16	0.45
2:B:290:SER:C	2:B:297:GLN:HE21	2.20	0.45
8:H:73:LEU:HD12	8:H:73:LEU:O	2.17	0.45
3:P:72:ARG:HH11	3:P:72:ARG:HG2	1.82	0.45
1:N:10:ASN:ND2	2:O:18:CYS:HB3	2.08	0.45
1:N:106:MET:N	1:N:107:PRO:HD2	2.32	0.45
5:E:81:ILE:HG22	5:E:100:HIS:HB2	1.99	0.45
9:I:70:LEU:CG	9:I:71:ASN:N	2.78	0.45
2:O:57:TYR:HE2	2:O:203:ARG:NH2	2.11	0.45
1:A:111:GLU:HG3	1:A:215:HIS:NE2	2.31	0.45
3:P:107:SER:OG	12:P:502:HEM:O1D	2.32	0.45
4:D:195:GLU:HG3	4:D:195:GLU:O	2.17	0.45
4:Q:37:CYS:C	4:Q:39:ALA:H	2.20	0.45
7:G:24:ARG:HB2	7:G:27:PRO:HB3	1.99	0.45
1:N:106:MET:HE2	1:N:110:VAL:CG2	2.47	0.44
1:N:106:MET:HE2	1:N:110:VAL:HG23	1.99	0.44
4:Q:178:THR:HG21	8:U:15:ASP:HA	1.99	0.44
2:O:290:SER:C	2:O:297:GLN:HE21	2.20	0.44
1:A:48:GLU:CD	1:A:54:GLY:H	2.21	0.44
2:B:162:ASN:O	2:B:244:ILE:HD12	2.17	0.44
1:N:282:ARG:HH21	9:V:36:UNK:HA	1.82	0.44
2:O:96:LEU:HD13	2:O:109:VAL:CG1	2.38	0.44
2:B:71:LEU:CD2	9:I:68:ILE:HG13	2.47	0.44
2:O:52:LYS:HB2	2:O:203:ARG:HB3	1.99	0.44
3:P:108:TYR:HB3	3:P:114:TRP:CE3	2.52	0.44
7:G:29:ILE:HA	7:G:33:ALA:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:181:GLU:HG2	5:E:182:VAL:N	2.31	0.44
6:F:71:LYS:O	6:F:72:HIS:HB2	2.16	0.44
5:R:153:PHE:C	5:R:155:GLY:H	2.20	0.44
3:C:187:PRO:HG2	12:C:501:HEM:HMC3	2.00	0.44
2:B:50:PHE:C	2:B:51:ILE:HG13	2.37	0.44
5:E:106:ILE:O	5:E:106:ILE:HG22	2.17	0.44
2:O:307:PHE:H	9:V:52:ARG:HG2	1.82	0.44
4:Q:26:VAL:HG12	4:Q:55:THR:HG21	1.99	0.44
2:B:101:THR:OG1	2:B:104:LYS:HG3	2.17	0.44
2:O:221:GLU:C	2:O:223:PHE:H	2.20	0.44
2:B:248:ASN:ND2	2:B:428:GLY:HA2	2.30	0.44
1:N:18:THR:HG23	1:N:24:ARG:CG	2.48	0.44
1:N:270:LEU:HA	1:N:270:LEU:HD23	1.81	0.44
4:D:151:PRO:HA	4:D:156:GLN:HG3	1.97	0.44
4:Q:116:ILE:HG21	4:Q:190:LEU:HD13	2.00	0.44
3:P:223:PRO:O	3:P:227:PHE:HB2	2.17	0.44
5:R:141:HIS:HB3	19:R:501:FES:S2	2.58	0.44
2:B:56:ARG:NH1	2:B:171:ALA:HB1	2.32	0.44
5:R:136:VAL:HG12	5:R:138:VAL:HG23	1.99	0.44
2:O:200:THR:OG1	2:O:203:ARG:HG3	2.17	0.44
1:A:253:VAL:O	1:A:323:HIS:HA	2.17	0.44
2:O:209:ILE:HD11	2:O:378:LEU:HG	2.00	0.44
4:Q:27:ARG:CZ	10:W:59:TYR:CE2	3.00	0.44
4:D:224:ARG:HH21	7:G:26:ILE:HA	1.81	0.44
2:B:366:ALA:O	2:B:367:THR:C	2.55	0.44
8:H:59:PHE:O	8:H:60:ASP:C	2.55	0.44
3:P:81:ARG:O	3:P:81:ARG:HD3	2.18	0.44
2:O:19:PRO:HG3	2:O:41:PHE:CD2	2.52	0.44
5:E:102:THR:O	5:E:103:GLN:HG3	2.17	0.44
2:B:22:GLU:HG3	2:B:23:ASP:N	2.32	0.44
1:N:23:LEU:HA	1:N:192:ALA:O	2.17	0.44
5:E:161:HIS:HB2	19:E:501:FES:S1	2.58	0.44
1:A:373:THR:N	1:A:374:PRO:HD2	2.31	0.44
2:B:368:TYR:O	2:B:372:VAL:HG23	2.18	0.44
2:B:76:THR:HG22	2:B:81:SER:CA	2.45	0.44
2:O:33:LEU:HD21	2:O:224:LEU:HD12	2.00	0.44
2:O:58:GLU:OE1	2:O:63:LEU:HA	2.18	0.44
5:R:185:TYR:HD2	5:R:185:TYR:N	2.16	0.44
2:B:63:LEU:O	2:B:182:ARG:NE	2.43	0.44
1:A:7:THR:HG21	2:B:113:ARG:CD	2.44	0.44
2:O:276:GLN:HG2	2:O:281:ALA:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:37:LEU:HD21	3:C:233:LEU:HA	1.98	0.44
8:H:17:LEU:HD13	8:H:73:LEU:CD2	2.47	0.44
3:P:282:LEU:HD12	3:P:291:GLY:C	2.38	0.44
4:D:116:ILE:HG21	4:D:190:LEU:HD13	2.00	0.44
4:D:239:PRO:C	4:D:241:LYS:H	2.20	0.44
4:D:75:ASP:O	4:Q:99:GLU:HG2	2.18	0.44
1:A:79:VAL:O	1:A:82:MET:HG2	2.17	0.44
2:O:101:THR:HG23	2:O:104:LYS:HE3	2.00	0.44
3:P:45:GLN:HB3	12:P:501:HEM:HAB	2.00	0.43
2:O:399:ALA:CA	2:O:402:ILE:HG22	2.47	0.43
3:P:287:ASN:O	3:P:288:LYS:C	2.55	0.43
3:P:216:SER:HB3	6:S:59:MET:HE1	2.00	0.43
3:C:378:LEU:HD22	6:F:33:ARG:HG3	2.01	0.43
1:A:418:LYS:O	1:A:420:PRO:HD3	2.18	0.43
7:G:56:TYR:O	7:G:59:TYR:HB3	2.18	0.43
5:E:189:GLY:O	5:E:192:LEU:O	2.35	0.43
2:O:385:GLU:C	2:O:387:LEU:N	2.72	0.43
2:B:276:GLN:HG2	2:B:281:ALA:HB2	1.99	0.43
1:A:289:HIS:O	1:A:290:LEU:C	2.57	0.43
2:B:156:GLN:HE22	9:I:77:ARG:C	2.21	0.43
2:B:67:HIS:O	2:B:70:ARG:HB3	2.18	0.43
2:B:39:GLU:OE2	2:B:113:ARG:NH2	2.50	0.43
9:V:32:UNK:N	9:V:73:PRO:HG2	2.32	0.43
2:B:379:LEU:O	2:B:379:LEU:HG	2.18	0.43
4:D:208:MET:O	4:D:212:SER:HB2	2.18	0.43
1:A:47:TYR:CE2	1:A:231:LEU:HD11	2.54	0.43
2:O:174:ASN:HA	2:O:175:PRO:HD2	1.85	0.43
3:P:36:SER:O	3:P:40:VAL:HG23	2.19	0.43
2:O:280:GLY:HA3	2:O:293:SER:OG	2.18	0.43
6:S:40:ASP:C	6:S:40:ASP:OD1	2.57	0.43
2:O:151:ALA:O	2:O:157:VAL:HG11	2.19	0.43
14:Q:3003:CDL:H721	14:Q:3003:CDL:HA62	1.99	0.43
4:D:91:PHE:HA	4:D:92:PRO:HD3	1.73	0.43
2:O:366:ALA:O	2:O:367:THR:C	2.57	0.43
2:O:338:ARG:NH1	2:O:338:ARG:CG	2.82	0.43
5:R:155:GLY:HA3	5:R:165:TYR:O	2.18	0.43
2:B:206:LEU:CG	2:B:216:LEU:HD11	2.47	0.43
1:A:295:ALA:O	1:A:298:ALA:HB3	2.18	0.43
3:C:362:ILE:HA	3:C:366:LEU:HB2	2.01	0.43
3:P:31:TRP:NE1	15:P:3007:PEE:O4	2.50	0.43
4:Q:68:VAL:HG12	4:Q:69:GLU:N	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:306:PRO:HA	9:I:52:ARG:HG2	1.99	0.43
3:P:50:LEU:O	3:P:54:MET:HG3	2.17	0.43
17:D:501:HEC:HBB3	17:D:501:HEC:HMB1	2.00	0.43
2:B:402:ILE:HG23	2:B:403:ASP:H	1.83	0.43
1:A:272:VAL:O	1:A:275:ALA:HB3	2.18	0.43
3:P:142:TRP:CD1	3:P:266:PRO:HD3	2.53	0.43
3:C:304:LEU:O	3:C:305:ILE:C	2.57	0.43
3:P:321:LEU:HB2	3:P:374:GLU:OE1	2.18	0.43
1:N:236:PHE:HB2	1:N:258:GLU:OE1	2.19	0.43
2:B:168:TYR:CB	2:B:173:ALA:HB2	2.40	0.43
1:N:240:GLU:HA	1:N:422:LEU:O	2.18	0.43
4:Q:57:THR:HG22	4:Q:58:GLU:N	2.32	0.43
4:Q:220:TYR:CE2	14:Q:3003:CDL:H722	2.54	0.43
1:A:177:LEU:HA	1:A:177:LEU:HD23	1.90	0.43
3:P:2:ALA:HB3	3:P:8:SER:HB3	2.00	0.43
1:A:361:LEU:O	1:A:364:ALA:HB3	2.17	0.43
1:N:344:ARG:HG3	1:N:344:ARG:HH11	1.83	0.43
2:O:295:LEU:O	2:O:299:VAL:HG23	2.19	0.43
5:E:101:ARG:HG2	5:E:105:GLU:CD	2.38	0.43
2:B:57:TYR:HD1	2:B:57:TYR:N	2.16	0.43
1:A:140:GLU:HG2	9:I:50:LEU:HG	1.99	0.43
3:C:313:GLN:HE21	6:F:36:THR:CB	2.31	0.43
2:B:207:VAL:HG21	2:B:383:GLY:HA2	2.01	0.43
2:O:207:VAL:HG21	2:O:383:GLY:HA2	2.00	0.43
3:P:285:ILE:HD12	3:P:294:ALA:HB2	2.00	0.43
6:F:52:GLU:HG3	6:F:56:ASN:ND2	2.34	0.43
1:A:41:ILE:HG22	1:A:42:GLY:N	2.34	0.43
3:P:38:LEU:HD23	3:P:38:LEU:HA	1.86	0.43
4:Q:208:MET:C	4:Q:208:MET:SD	2.97	0.43
5:R:135:LEU:CD2	5:R:182:VAL:HG22	2.49	0.43
1:N:18:THR:HG23	1:N:24:ARG:HG3	2.00	0.43
3:P:313:GLN:HE21	6:S:36:THR:CB	2.32	0.43
4:Q:27:ARG:NH1	4:Q:55:THR:O	2.46	0.43
4:Q:116:ILE:HG23	4:Q:117:VAL:N	2.34	0.43
3:P:172:ASP:C	3:P:174:PRO:HD2	2.39	0.43
1:N:433:ASP:OD1	1:N:435:ASN:HB2	2.18	0.43
2:O:135:TRP:O	2:O:136:GLU:C	2.57	0.43
3:C:273:TRP:CD2	3:C:274:TYR:N	2.87	0.43
3:P:72:ARG:NE	4:Q:115:TYR:OH	2.52	0.43
5:R:77:LYS:HA	5:R:192:LEU:HD23	2.01	0.43
4:D:223:LYS:HD3	4:D:223:LYS:C	2.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:69:LYS:HD2	1:N:70:ARG:HH21	1.83	0.43
7:T:50:PRO:HB2	7:T:51:PRO:HD2	1.99	0.43
3:C:342:GLN:HB3	3:C:348:PHE:CE1	2.54	0.43
3:P:22:LEU:HD12	3:P:23:PRO:N	2.34	0.43
5:R:86:ASN:OD1	5:R:99:ARG:HB2	2.19	0.43
3:P:198:LEU:HD21	12:P:502:HEM:CMA	2.49	0.43
3:P:279:TYR:O	3:P:282:LEU:HB3	2.18	0.43
10:J:57:HIS:ND1	10:J:58:LYS:N	2.67	0.43
3:C:247:SER:OG	3:C:250:LEU:HB2	2.19	0.43
2:O:264:VAL:HG12	2:O:265:GLY:N	2.34	0.43
4:D:165:TYR:O	4:D:166:ASN:C	2.57	0.43
3:P:41:CYS:SG	3:P:91:PHE:HA	2.58	0.43
1:A:178:THR:O	1:A:179:ARG:C	2.58	0.42
2:O:124:LEU:HD23	2:O:124:LEU:C	2.39	0.42
5:E:130:PRO:O	5:E:132:TRP:N	2.52	0.42
1:N:27:SER:HA	1:N:199:ALA:O	2.19	0.42
5:R:134:ILE:HB	5:R:185:TYR:CE1	2.54	0.42
5:R:171:ILE:HG22	5:R:179:ASN:OD1	2.19	0.42
2:B:209:ILE:HD11	2:B:378:LEU:HG	2.01	0.42
3:P:342:GLN:HB3	3:P:348:PHE:CE1	2.54	0.42
1:N:106:MET:CE	1:N:110:VAL:HG21	2.49	0.42
13:P:3002:UQ:HM51	13:P:3002:UQ:H8	2.01	0.42
7:T:29:ILE:HA	7:T:33:ALA:HB3	2.00	0.42
3:P:325:LEU:HD12	3:P:325:LEU:HA	1.77	0.42
3:C:329:LEU:O	3:C:332:ASN:HB3	2.20	0.42
8:U:27:THR:O	8:U:31:VAL:HG23	2.19	0.42
6:S:70:LEU:HD12	6:S:70:LEU:O	2.19	0.42
1:N:404:ALA:O	1:N:406:MET:N	2.53	0.42
1:A:433:ASP:CG	1:A:435:ASN:HB2	2.39	0.42
4:D:178:THR:HG21	8:H:15:ASP:HA	2.00	0.42
13:C:2002:UQ:HM51	13:C:2002:UQ:H8	2.01	0.42
1:A:165:ARG:HG3	1:A:165:ARG:NH1	2.35	0.42
3:P:145:THR:O	3:P:149:ASN:HB2	2.20	0.42
3:C:336:LEU:HA	3:C:336:LEU:HD23	1.86	0.42
2:O:96:LEU:HB3	9:V:70:LEU:HD22	2.01	0.42
2:O:172:LEU:HD13	2:O:316:TYR:CD1	2.54	0.42
2:O:357:VAL:O	2:O:361:LYS:HG3	2.19	0.42
3:P:362:ILE:HA	3:P:366:LEU:HB2	2.00	0.42
1:A:45:SER:HA	1:A:48:GLU:CD	2.39	0.42
2:O:162:ASN:O	2:O:244:ILE:HD12	2.19	0.42
3:C:333:LEU:HD21	3:C:359:TYR:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:178:THR:O	1:N:179:ARG:C	2.58	0.42
1:A:37:VAL:HG22	1:A:109:VAL:HG11	2.01	0.42
3:P:325:LEU:HD22	3:P:370:ILE:HG13	2.02	0.42
2:O:206:LEU:HG	2:O:216:LEU:HD11	2.01	0.42
1:N:289:HIS:O	1:N:290:LEU:C	2.58	0.42
5:R:161:HIS:HB2	19:R:501:FES:S1	2.59	0.42
2:B:163:LEU:O	2:B:166:ALA:N	2.49	0.42
8:U:28:GLU:O	8:U:32:LYS:HG3	2.19	0.42
2:B:355:GLU:O	2:B:358:THR:N	2.52	0.42
2:O:341:MET:HE2	2:O:341:MET:CA	2.49	0.42
2:B:144:LEU:CB	2:B:183:ILE:HD12	2.42	0.42
3:C:377:MET:CE	6:F:20:TYR:HB2	2.50	0.42
2:B:341:MET:CE	2:B:417:PHE:CE2	2.93	0.42
3:P:277:PHE:CG	3:P:278:ALA:N	2.88	0.42
1:N:402:VAL:HG22	1:N:406:MET:HE2	1.98	0.42
5:R:99:ARG:HB3	5:R:133:VAL:HG12	2.02	0.42
2:O:257:VAL:HG22	2:O:424:MET:HG3	2.02	0.42
1:A:365:MET:HG3	1:A:366:VAL:N	2.35	0.42
3:P:377:MET:CE	6:S:20:TYR:HB2	2.50	0.42
7:T:34:LEU:HB2	7:T:35:PRO:HD3	2.02	0.42
2:O:26:ILE:HG23	2:O:26:ILE:O	2.19	0.42
1:A:281:ASP:OD2	9:I:33:UNK:HB2	2.18	0.42
2:B:341:MET:HE2	2:B:341:MET:HA	2.02	0.42
2:B:51:ILE:CG2	2:B:52:LYS:N	2.82	0.42
1:N:394:GLU:O	1:N:395:TRP:C	2.58	0.42
3:C:245:LEU:O	4:D:201:ARG:HD2	2.19	0.42
5:R:141:HIS:O	5:R:142:LEU:HD23	2.19	0.42
6:S:52:GLU:HG3	6:S:56:ASN:ND2	2.35	0.42
2:O:221:GLU:O	2:O:223:PHE:N	2.51	0.42
1:A:106:MET:HE2	1:A:110:VAL:HG23	2.02	0.42
3:P:186:LEU:O	3:P:187:PRO:C	2.58	0.42
5:R:76:ILE:CD1	5:R:98:VAL:HG21	2.50	0.42
7:G:29:ILE:HA	7:G:33:ALA:CB	2.50	0.42
1:A:331:ILE:CG2	1:A:431:LEU:HB2	2.46	0.42
2:O:306:PRO:HB3	9:V:52:ARG:H	1.85	0.42
2:B:133:ARG:HD3	2:B:135:TRP:CZ2	2.55	0.42
2:B:266:SER:HB3	2:B:269:ALA:HB2	2.01	0.42
1:A:228:VAL:HG13	1:A:228:VAL:O	2.20	0.42
2:O:314:VAL:HG22	9:V:63:ASP:N	2.34	0.42
3:P:187:PRO:HG2	12:P:501:HEM:HMC3	2.00	0.42
5:E:190:ASP:C	5:E:192:LEU:N	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:VAL:HG22	1:A:406:MET:HE2	2.01	0.42
3:C:279:TYR:O	3:C:282:LEU:HB3	2.19	0.42
4:D:134:TYR:CG	4:D:162:PRO:HG3	2.55	0.42
2:O:366:ALA:O	2:O:369:LEU:N	2.52	0.42
4:D:197:GLU:O	4:D:198:HIS:C	2.58	0.42
4:D:26:VAL:HG22	4:D:188:THR:HG22	2.02	0.42
2:O:408:ALA:O	2:O:409:ASP:C	2.57	0.42
4:Q:165:TYR:O	4:Q:166:ASN:C	2.58	0.42
2:O:259:THR:O	2:O:260:GLU:C	2.56	0.42
2:O:268:GLU:HG2	2:O:268:GLU:O	2.20	0.42
2:B:264:VAL:HG23	2:B:316:TYR:O	2.20	0.41
2:O:63:LEU:HB2	2:O:182:ARG:CD	2.46	0.41
5:R:76:ILE:HD13	5:R:89:PHE:CD1	2.54	0.41
1:N:146:THR:O	1:N:150:PHE:HD1	2.03	0.41
1:N:331:ILE:CG2	1:N:431:LEU:HB2	2.47	0.41
2:B:385:GLU:C	2:B:387:LEU:N	2.72	0.41
1:N:365:MET:HG3	1:N:366:VAL:N	2.35	0.41
1:N:219:VAL:CG1	1:N:220:SER:N	2.83	0.41
5:E:177:PRO:HG2	5:E:178:TYR:H	1.85	0.41
5:R:35:PHE:O	5:R:38:LEU:HB3	2.19	0.41
2:B:192:HIS:O	2:B:196:GLN:HG3	2.19	0.41
1:A:205:HIS:O	1:A:208:LEU:HB3	2.20	0.41
2:O:176:LEU:O	2:O:176:LEU:HD12	2.20	0.41
5:E:37:TYR:CE2	15:E:2005:PEE:H10	2.56	0.41
8:U:59:PHE:O	8:U:60:ASP:C	2.58	0.41
2:O:35:ILE:O	2:O:213:HIS:HE1	2.03	0.41
2:B:29:LEU:HB3	2:B:30:PRO:HD2	2.02	0.41
4:Q:26:VAL:HG22	4:Q:188:THR:HG22	2.02	0.41
10:J:60:GLU:HA	10:J:60:GLU:OE2	2.20	0.41
14:C:2004:CDL:HA32	7:G:40:ARG:HB3	2.02	0.41
3:C:120:LEU:HD23	3:C:120:LEU:HA	1.87	0.41
1:A:21:ASN:N	1:A:21:ASN:OD1	2.54	0.41
6:S:67:ASP:HA	6:S:70:LEU:HD23	2.02	0.41
5:R:97:PHE:O	5:R:134:ILE:HA	2.20	0.41
5:E:86:ASN:HD22	5:E:148:ALA:CB	2.30	0.41
3:P:245:LEU:HD23	3:P:245:LEU:HA	1.90	0.41
4:Q:229:VAL:CG2	7:T:20:PRO:HG3	2.50	0.41
4:Q:91:PHE:HA	4:Q:92:PRO:HD3	1.75	0.41
3:C:223:PRO:O	3:C:227:PHE:HB2	2.20	0.41
6:S:32:MET:O	6:S:33:ARG:C	2.58	0.41
2:B:287:ARG:CB	9:I:53:GLU:HG3	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:LYS:O	1:A:195:MET:HG3	2.21	0.41
2:O:85:ILE:HA	2:O:122:TYR:CD2	2.56	0.41
8:U:15:ASP:C	8:U:17:LEU:N	2.74	0.41
2:B:345:LYS:HG2	2:B:418:VAL:HG11	2.02	0.41
6:F:58:ARG:HD2	6:F:89:TYR:OH	2.21	0.41
1:N:10:ASN:ND2	2:O:19:PRO:CD	2.84	0.41
6:S:70:LEU:HD12	6:S:70:LEU:C	2.41	0.41
1:N:41:ILE:HD13	1:N:190:PHE:CD2	2.55	0.41
4:Q:237:TYR:HB2	6:S:60:PHE:CD2	2.55	0.41
2:O:206:LEU:CD2	2:O:220:ALA:HB2	2.51	0.41
1:A:58:PHE:HZ	1:A:131:ARG:HB2	1.86	0.41
3:P:64:PHE:CD2	3:P:259:PRO:HG3	2.56	0.41
5:E:122:HIS:HB3	5:E:125:ASP:CG	2.41	0.41
1:A:220:SER:HB2	1:A:225:GLU:HB2	2.03	0.41
2:B:172:LEU:HD13	2:B:316:TYR:CD1	2.55	0.41
9:V:70:LEU:HD21	9:V:71:ASN:OD1	2.20	0.41
1:N:429:GLU:OE2	7:T:7:LEU:HB2	2.21	0.41
3:C:321:LEU:HB2	3:C:374:GLU:OE1	2.21	0.41
4:D:102:ARG:NH1	4:D:102:ARG:HG2	2.36	0.41
2:B:280:GLY:HA3	2:B:293:SER:HG	1.86	0.41
1:N:294:LEU:HD23	1:N:307:PHE:CZ	2.56	0.41
3:P:28:ILE:HG13	3:P:225:TYR:CE2	2.56	0.41
4:Q:221:TYR:HD2	5:R:39:VAL:HG11	1.84	0.41
4:Q:37:CYS:O	4:Q:39:ALA:N	2.54	0.41
1:A:172:GLU:O	1:A:175:LYS:N	2.51	0.41
4:Q:110:PRO:HA	4:Q:111:PRO:HD2	1.93	0.41
1:A:89:TYR:CD1	1:A:89:TYR:C	2.94	0.41
2:B:222:GLN:O	2:B:222:GLN:CG	2.68	0.41
2:B:314:VAL:HG11	2:B:316:TYR:CZ	2.55	0.41
9:V:33:UNK:N	9:V:73:PRO:CG	2.83	0.41
5:E:77:LYS:HA	5:E:192:LEU:HD23	2.01	0.41
3:C:245:LEU:HD23	3:C:245:LEU:HA	1.88	0.41
8:H:15:ASP:C	8:H:17:LEU:N	2.74	0.41
1:N:191:LYS:N	1:N:195:MET:HE2	2.36	0.41
4:D:204:MET:HE3	18:D:2009:BOG:H1'1	2.02	0.41
1:A:34:THR:HA	1:A:102:LEU:HA	2.02	0.41
1:A:69:LYS:HD2	1:A:70:ARG:HH21	1.85	0.41
2:O:47:ILE:CG2	2:O:48:GLY:N	2.84	0.41
2:B:248:ASN:HA	2:O:181:TYR:CD2	2.55	0.41
2:O:56:ARG:HA	2:O:171:ALA:O	2.20	0.41
1:N:206:LYS:H	1:N:206:LYS:HD2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:438:ARG:NH1	1:A:438:ARG:HG3	2.35	0.41
2:B:307:PHE:HD1	2:B:308:ASP:N	2.19	0.41
6:F:13:MET:HE1	6:F:16:ILE:HD12	2.03	0.41
2:O:169:LYS:HG3	2:O:240:TRP:HB2	2.01	0.41
5:E:97:PHE:O	5:E:134:ILE:HA	2.21	0.41
1:A:280:TYR:CD2	1:A:281:ASP:N	2.88	0.41
9:I:31:UNK:CA	9:I:73:PRO:HG2	2.51	0.41
6:S:67:ASP:CG	6:S:71:LYS:HZ3	2.24	0.41
1:A:106:MET:HE2	1:A:110:VAL:CG2	2.50	0.41
2:B:56:ARG:HA	2:B:171:ALA:O	2.21	0.41
5:R:122:HIS:HA	5:R:170:ARG:NH1	2.36	0.41
7:G:41:PHE:CE2	7:G:45:VAL:HG21	2.56	0.41
1:A:404:ALA:O	1:A:405:ARG:C	2.59	0.41
8:U:17:LEU:HD13	8:U:73:LEU:CD2	2.48	0.41
3:C:18:SER:HB2	3:C:202:HIS:HE1	1.85	0.41
1:N:433:ASP:CG	1:N:435:ASN:HB2	2.41	0.41
1:N:351:GLU:O	1:N:354:VAL:HG22	2.21	0.41
6:S:31:LEU:HD21	6:S:65:ALA:CB	2.51	0.41
2:B:133:ARG:HA	2:B:134:PRO:HD3	1.91	0.41
4:Q:37:CYS:C	4:Q:39:ALA:N	2.74	0.41
4:D:40:CYS:SG	17:D:501:HEC:HMC1	2.61	0.41
2:B:325:TYR:CD1	9:I:60:ALA:HB3	2.56	0.41
4:Q:29:GLY:HA3	4:Q:189:PHE:HB2	2.03	0.41
2:B:59:THR:O	2:B:61:ALA:N	2.53	0.41
4:Q:54:VAL:HG11	4:Q:192:TRP:NE1	2.35	0.41
1:N:243:ALA:O	1:N:425:VAL:HA	2.20	0.41
4:D:28:ARG:O	4:D:31:GLN:N	2.54	0.41
3:P:47:LEU:HD12	3:P:47:LEU:HA	1.93	0.41
3:C:328:LEU:CD1	7:G:51:PRO:HB3	2.38	0.41
2:B:23:ASP:O	2:B:24:LEU:CB	2.56	0.41
1:N:281:ASP:C	1:N:283:THR:H	2.24	0.41
5:E:141:HIS:HB2	5:E:176:ALA:HB2	2.03	0.41
4:Q:240:PRO:O	4:Q:241:LYS:OXT	2.39	0.41
3:C:142:TRP:CD1	3:C:266:PRO:HD3	2.56	0.41
1:N:305:HIS:HB3	9:V:36:UNK:CB	2.51	0.41
1:A:47:TYR:CZ	1:A:231:LEU:HD11	2.56	0.41
4:D:215:LEU:HD13	5:E:46:ALA:HB3	2.03	0.41
1:A:351:GLU:O	1:A:354:VAL:HG22	2.21	0.41
1:N:264:ASP:HA	1:N:265:PRO:HD3	1.84	0.41
10:W:10:TYR:C	10:W:10:TYR:CD2	2.94	0.41
9:V:33:UNK:N	9:V:73:PRO:HG2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:7:THR:HG21	2:O:113:ARG:CD	2.47	0.40
1:A:433:ASP:OD1	1:A:435:ASN:HB2	2.21	0.40
3:C:246:PHE:O	3:C:248:PRO:HD3	2.21	0.40
6:S:82:LYS:O	6:S:83:TYR:C	2.58	0.40
4:D:70:VAL:HG21	4:D:83:ARG:CZ	2.52	0.40
1:N:439:SER:C	1:N:441:MET:H	2.24	0.40
1:A:106:MET:N	1:A:107:PRO:HD2	2.36	0.40
9:I:38:UNK:C	9:I:40:UNK:N	2.64	0.40
3:P:23:PRO:HG2	7:T:3:HIS:HB3	2.03	0.40
3:P:92:PHE:CA	3:P:95:ILE:HG22	2.49	0.40
2:O:159:VAL:HG21	2:O:325:TYR:CE1	2.55	0.40
6:S:57:GLU:O	6:S:61:ARG:HG3	2.21	0.40
1:N:439:SER:HA	1:N:442:TYR:CE2	2.56	0.40
1:N:159:GLN:NE2	5:R:7:VAL:HG11	2.37	0.40
8:U:36:ARG:HB3	8:U:36:ARG:CZ	2.51	0.40
5:R:83:GLU:HA	5:R:100:HIS:CB	2.49	0.40
2:B:198:ASN:HA	2:B:203:ARG:NH1	2.37	0.40
5:E:136:VAL:CG2	5:E:183:PRO:HD3	2.45	0.40
2:B:209:ILE:HD12	2:B:379:LEU:HB2	2.03	0.40
5:E:99:ARG:HB3	5:E:133:VAL:HG12	2.03	0.40
1:N:134:ILE:HG21	1:N:174:ILE:CD1	2.50	0.40
4:D:167:GLU:HG3	8:H:13:LEU:CD2	2.50	0.40
3:C:22:LEU:HD12	3:C:23:PRO:HD2	2.03	0.40
8:H:44:VAL:HG21	8:H:54:CYS:SG	2.61	0.40
1:A:293:ARG:CD	1:A:344:ARG:CZ	3.00	0.40
1:N:220:SER:HB2	1:N:225:GLU:HB2	2.03	0.40
2:O:101:THR:OG1	2:O:104:LYS:HG3	2.21	0.40
17:D:501:HEC:HMC1	17:D:501:HEC:HBC3	2.04	0.40
3:P:75:GLN:O	3:P:76:TYR:HB2	2.21	0.40
1:A:204:SER:HB3	1:A:207:GLU:HB2	2.03	0.40
5:E:101:ARG:HD2	5:E:105:GLU:HB3	2.03	0.40
2:B:56:ARG:NH2	2:B:318:ASP:OD2	2.55	0.40
2:B:51:ILE:HG22	2:B:52:LYS:N	2.37	0.40
1:A:296:ALA:O	1:A:299:VAL:N	2.55	0.40
2:O:368:TYR:O	2:O:372:VAL:HG23	2.21	0.40
5:E:52:LYS:CD	5:E:52:LYS:C	2.89	0.40
1:A:270:LEU:HA	1:A:270:LEU:HD23	1.88	0.40
1:N:45:SER:HA	1:N:48:GLU:CD	2.41	0.40
4:D:26:VAL:HG12	4:D:55:THR:HG21	2.03	0.40
5:R:30:GLU:HB2	10:W:7:ARG:HG3	2.03	0.40
3:C:130:VAL:HG23	3:C:131:GLY:N	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:388:LEU:O	2:O:389:SER:HB2	2.21	0.40
3:C:38:LEU:HD23	3:C:38:LEU:HA	1.78	0.40
5:E:130:PRO:C	5:E:132:TRP:N	2.75	0.40
5:R:165:TYR:CD2	5:R:180:LEU:HG	2.57	0.40
2:B:62:ASN:O	2:B:65:THR:CG2	2.64	0.40
3:C:22:LEU:HD12	3:C:23:PRO:CD	2.51	0.40
3:C:172:ASP:C	3:C:174:PRO:HD2	2.42	0.40
2:O:80:ALA:HA	2:O:84:ARG:HH12	1.85	0.40
2:O:227:ARG:HB3	2:O:228:SER:H	1.42	0.40
2:O:29:LEU:HB3	2:O:30:PRO:HD2	2.03	0.40
3:P:51:LEU:HD23	3:P:51:LEU:HA	1.88	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%)	384 (87%)	48 (11%)	9 (2%)	9	46
1	N	440/446 (99%)	385 (88%)	45 (10%)	10 (2%)	8	42
2	B	419/441 (95%)	350 (84%)	51 (12%)	18 (4%)	3	23
2	O	420/441 (95%)	359 (86%)	46 (11%)	15 (4%)	4	28
3	C	378/380 (100%)	346 (92%)	25 (7%)	7 (2%)	10	48
3	P	377/380 (99%)	336 (89%)	33 (9%)	8 (2%)	9	44
4	D	239/241 (99%)	218 (91%)	17 (7%)	4 (2%)	11	50
4	Q	239/241 (99%)	216 (90%)	17 (7%)	6 (2%)	7	39
5	E	194/196 (99%)	148 (76%)	30 (16%)	16 (8%)	1	6
5	R	194/196 (99%)	162 (84%)	27 (14%)	5 (3%)	7	38
6	F	99/110 (90%)	93 (94%)	6 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	S	99/110 (90%)	89 (90%)	10 (10%)	0	100	100
7	G	78/81 (96%)	65 (83%)	11 (14%)	2 (3%)	7	38
7	T	77/81 (95%)	65 (84%)	10 (13%)	2 (3%)	7	38
8	H	68/77 (88%)	59 (87%)	9 (13%)	0	100	100
8	U	65/77 (84%)	53 (82%)	12 (18%)	0	100	100
9	I	29/47 (62%)	26 (90%)	3 (10%)	0	100	100
9	V	29/47 (62%)	23 (79%)	6 (21%)	0	100	100
10	J	59/61 (97%)	53 (90%)	5 (8%)	1 (2%)	11	50
10	W	58/61 (95%)	51 (88%)	7 (12%)	0	100	100
All	All	4002/4160 (96%)	3481 (87%)	418 (10%)	103 (3%)	7	38

All (103) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	282	ARG
2	B	26	ILE
2	B	29	LEU
2	B	171	ALA
2	B	224	LEU
2	B	227	ARG
3	C	287	ASN
5	E	115	SER
5	E	128	LYS
5	E	130	PRO
5	E	163	SER
5	E	191	ASP
1	N	282	ARG
1	N	433	ASP
2	O	19	PRO
2	O	26	ILE
2	O	171	ALA
2	O	228	SER
3	P	287	ASN
1	A	71	PRO
1	A	218	GLY
1	A	405	ARG
1	A	433	ASP
2	B	21	ALA
2	B	201	SER

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Mol	Chain	Res	Type
2	B	221	GLU
2	B	372	VAL
2	B	386	ALA
2	B	389	SER
5	E	102	THR
5	E	127	VAL
5	E	131	GLU
5	E	137	GLY
2	O	24	LEU
2	O	201	SER
2	O	221	GLU
2	O	222	GLN
2	O	372	VAL
2	O	386	ALA
2	O	389	SER
3	P	274	TYR
5	R	137	GLY
5	R	154	GLY
5	R	163	SER
7	T	33	ALA
2	B	24	LEU
2	B	46	ARG
3	C	3	PRO
4	D	166	ASN
5	E	80	ASP
5	E	120	PRO
5	E	177	PRO
7	G	33	ALA
1	N	72	CYS
2	O	46	ARG
2	O	330	ALA
3	P	111	LYS
4	Q	166	ASN
4	Q	177	ALA
5	R	186	GLN
5	R	191	ASP
7	T	50	PRO
1	A	65	LYS
1	A	72	CYS
1	A	145	MET
2	B	189	GLU
3	C	111	LYS

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Mol	Chain	Res	Type
5	E	123	ASP
5	E	154	GLY
1	N	65	LYS
1	N	71	PRO
1	N	145	MET
1	N	262	TRP
1	N	405	ARG
3	P	156	TYR
3	P	264	VAL
2	B	319	SER
3	C	17	ASN
4	D	38	SER
4	D	176	PRO
7	G	50	PRO
10	J	61	ALA
2	O	404	SER
3	P	158	GLY
4	Q	38	SER
4	Q	176	PRO
4	Q	198	HIS
2	B	431	GLY
3	C	19	LEU
5	E	189	GLY
3	P	3	PRO
2	B	20	GLY
5	E	188	VAL
1	N	428	ILE
2	B	129	ALA
4	Q	162	PRO
3	C	158	GLY
3	C	264	VAL
1	N	218	GLY
3	P	157	ILE
1	A	428	ILE
4	D	162	PRO
2	O	431	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	365/368 (99%)	353 (97%)	12 (3%)	45	80
1	N	365/368 (99%)	352 (96%)	13 (4%)	42	78
2	B	332/347 (96%)	319 (96%)	13 (4%)	39	76
2	O	333/347 (96%)	319 (96%)	14 (4%)	36	74
3	C	328/329 (100%)	323 (98%)	5 (2%)	72	91
3	P	328/329 (100%)	322 (98%)	6 (2%)	66	89
4	D	200/200 (100%)	197 (98%)	3 (2%)	72	91
4	Q	200/200 (100%)	197 (98%)	3 (2%)	72	91
5	E	166/166 (100%)	163 (98%)	3 (2%)	66	89
5	R	165/166 (99%)	162 (98%)	3 (2%)	66	89
6	F	93/96 (97%)	90 (97%)	3 (3%)	46	81
6	S	93/96 (97%)	88 (95%)	5 (5%)	27	67
7	G	71/71 (100%)	69 (97%)	2 (3%)	51	83
7	T	70/71 (99%)	68 (97%)	2 (3%)	50	83
8	H	65/71 (92%)	64 (98%)	1 (2%)	72	91
8	U	63/71 (89%)	62 (98%)	1 (2%)	70	90
9	I	23/26 (88%)	21 (91%)	2 (9%)	13	44
9	V	23/26 (88%)	22 (96%)	1 (4%)	35	74
10	J	49/49 (100%)	47 (96%)	2 (4%)	37	75
10	W	47/49 (96%)	46 (98%)	1 (2%)	61	87
All	All	3379/3446 (98%)	3284 (97%)	95 (3%)	51	83

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	A	86	PHE
1	A	90	THR
1	A	106	MET
1	A	226	ASP
1	A	281	ASP
1	A	307	PHE
1	A	395	TRP

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Mol	Chain	Res	Type
1	A	405	ARG
1	A	422	LEU
1	A	432	LEU
1	A	443	TRP
2	B	31	ASN
2	B	38	LEU
2	B	57	TYR
2	B	97	SER
2	B	104	LYS
2	B	170	THR
2	B	193	HIS
2	B	228	SER
2	B	248	ASN
2	B	304	THR
2	B	341	MET
2	B	402	ILE
2	B	424	MET
3	C	69	HIS
3	C	81	ARG
3	C	223	PRO
3	C	259	PRO
3	C	367	PHE
4	D	43	MET
4	D	72	ASP
4	D	203	ARG
5	E	52	LYS
5	E	131	GLU
5	E	185	TYR
6	F	58	ARG
6	F	70	LEU
6	F	78	GLU
7	G	4	PHE
7	G	17	SER
8	H	71	HIS
9	I	70	LEU
9	I	71	ASN
10	J	59	TYR
10	J	60	GLU
1	N	18	THR
1	N	49	ASN
1	N	86	PHE
1	N	90	THR

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Mol	Chain	Res	Type
1	N	106	MET
1	N	281	ASP
1	N	307	PHE
1	N	395	TRP
1	N	405	ARG
1	N	420	PRO
1	N	422	LEU
1	N	432	LEU
1	N	443	TRP
2	O	19	PRO
2	O	31	ASN
2	O	38	LEU
2	O	57	TYR
2	O	59	THR
2	O	97	SER
2	O	104	LYS
2	O	170	THR
2	O	193	HIS
2	O	223	PHE
2	O	248	ASN
2	O	341	MET
2	O	402	ILE
2	O	424	MET
3	P	69	HIS
3	P	81	ARG
3	P	259	PRO
3	P	277	PHE
3	P	334	LEU
3	P	367	PHE
4	Q	43	MET
4	Q	72	ASP
4	Q	203	ARG
5	R	52	LYS
5	R	80	ASP
5	R	185	TYR
6	S	13	MET
6	S	58	ARG
6	S	70	LEU
6	S	78	GLU
6	S	84	GLU
7	T	4	PHE
7	T	27	PRO

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Mol	Chain	Res	Type
8	U	71	HIS
9	V	59	SER
10	W	59	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	49	ASN
1	A	85	HIS
1	A	274	ASN
1	A	289	HIS
1	A	301	HIS
1	A	308	GLN
1	A	339	GLN
2	B	31	ASN
2	B	153	GLN
2	B	156	GLN
2	B	247	GLN
2	B	248	ASN
2	B	276	GLN
2	B	329	GLN
2	B	343	GLN
3	C	9	HIS
3	C	17	ASN
3	C	73	ASN
3	C	82	ASN
3	C	149	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
5	E	3	ASN
5	E	57	GLN
5	E	122	HIS
5	E	149	ASN
5	E	164	HIS
6	F	56	ASN
7	G	6	ASN
7	G	23	GLN

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Mol	Chain	Res	Type
7	G	73	ASN
9	I	71	ASN
1	N	10	ASN
1	N	49	ASN
1	N	85	HIS
1	N	118	GLN
1	N	274	ASN
1	N	289	HIS
1	N	308	GLN
1	N	339	GLN
2	O	31	ASN
2	O	156	GLN
2	O	247	GLN
2	O	248	ASN
2	O	276	GLN
2	O	329	GLN
2	O	343	GLN
3	P	9	HIS
3	P	17	ASN
3	P	69	HIS
3	P	82	ASN
3	P	207	ASN
3	P	313	GLN
3	P	342	GLN
4	Q	35	GLN
4	Q	50	ASN
5	R	57	GLN
5	R	122	HIS
5	R	164	HIS
6	S	72	HIS
7	T	23	GLN
7	T	44	GLN
7	T	73	ASN
7	T	79	ASN
8	U	71	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 36 ligands modelled in this entry, 9 are unknown - leaving 27 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$
13	UQ	C	2002	-	19,19,63	2.57	11 (57%)	23,26,79	1.30	4 (17%)
14	CDL	C	2004	-	39,39,99	1.20	2 (5%)	41,51,111	1.18	4 (9%)
15	PEE	C	2007	-	48,48,50	1.32	6 (12%)	49,53,55	0.93	5 (10%)
15	PEE	C	2008	-	20,20,50	1.84	6 (30%)	21,25,55	0.67	0
16	GOL	C	2011	-	5,5,5	1.15	0	5,5,5	0.52	0
12	HEM	C	501	3	30,50,50	2.77	10 (33%)	24,82,82	2.65	12 (50%)
12	HEM	C	502	3	30,50,50	2.48	7 (23%)	24,82,82	2.15	6 (25%)
14	CDL	D	2003	-	41,41,99	1.14	1 (2%)	43,53,111	1.11	5 (11%)
18	BOG	D	2009	-	20,20,20	0.99	1 (5%)	25,25,25	0.93	1 (4%)
18	BOG	D	2091	-	13,13,20	1.38	2 (15%)	18,18,25	1.13	2 (11%)
17	HEC	D	501	4	24,50,50	3.45	3 (12%)	19,82,82	3.25	6 (31%)
15	PEE	E	2005	-	49,49,50	1.50	10 (20%)	50,54,55	0.94	5 (10%)
19	FES	E	501	5	0,4,4	0.00	-	0,4,4	0.00	-
15	PEE	N	3008	-	4,4,50	3.86	4 (100%)	6,6,55	0.55	0
18	BOG	P	2010	-	12,12,20	1.48	3 (25%)	17,17,25	0.66	0
13	UQ	P	3002	-	19,19,63	2.48	11 (57%)	23,26,79	1.34	4 (17%)
14	CDL	P	3004	-	39,39,99	1.18	3 (7%)	41,51,111	1.21	4 (9%)
15	PEE	P	3007	-	48,48,50	1.25	6 (12%)	49,53,55	0.87	4 (8%)
16	GOL	P	3011	-	5,5,5	1.24	0	5,5,5	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
12	HEM	P	501	3	30,50,50	3.25	11 (36%)	24,82,82	2.38	9 (37%)
12	HEM	P	502	3	30,50,50	2.59	9 (30%)	24,82,82	2.17	8 (33%)
14	CDL	Q	3003	-	41,41,99	1.13	1 (2%)	43,53,111	1.10	5 (11%)
18	BOG	Q	3009	-	20,20,20	0.94	1 (5%)	25,25,25	0.95	1 (4%)
18	BOG	Q	3091	-	13,13,20	1.39	3 (23%)	18,18,25	1.06	2 (11%)
17	HEC	Q	501	4	24,50,50	2.38	3 (12%)	19,82,82	3.30	6 (31%)
15	PEE	R	3005	-	49,49,50	1.44	10 (20%)	50,54,55	0.94	5 (10%)
19	FES	R	501	5	0,4,4	0.00	-	0,4,4	0.00	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	UQ	C	2002	-	-	0/11/35/87	0/1/1/1
14	CDL	C	2004	-	-	0/49/49/110	0/0/0/0
15	PEE	C	2007	-	-	0/52/52/54	0/0/0/0
15	PEE	C	2008	-	-	0/24/24/54	0/0/0/0
16	GOL	C	2011	-	-	0/4/4/4	0/0/0/0
12	HEM	C	501	3	-	0/10/54/54	0/0/8/8
12	HEM	C	502	3	-	0/10/54/54	0/0/8/8
14	CDL	D	2003	-	-	0/51/51/110	0/0/0/0
18	BOG	D	2009	-	-	0/11/31/31	0/1/1/1
18	BOG	D	2091	-	-	0/4/24/31	0/1/1/1
17	HEC	D	501	4	-	0/6/54/54	0/0/8/8
15	PEE	E	2005	-	-	0/53/53/54	0/0/0/0
19	FES	E	501	5	-	0/0/4/4	0/1/1/1
15	PEE	N	3008	-	-	0/0/0/54	0/0/0/0
18	BOG	P	2010	-	-	0/2/22/31	0/1/1/1
13	UQ	P	3002	-	-	0/11/35/87	0/1/1/1
14	CDL	P	3004	-	-	0/49/49/110	0/0/0/0
15	PEE	P	3007	-	-	0/52/52/54	0/0/0/0
16	GOL	P	3011	-	-	0/4/4/4	0/0/0/0
12	HEM	P	501	3	-	0/10/54/54	0/0/8/8
12	HEM	P	502	3	-	0/10/54/54	0/0/8/8
14	CDL	Q	3003	-	-	0/51/51/110	0/0/0/0
18	BOG	Q	3009	-	-	0/11/31/31	0/1/1/1
18	BOG	Q	3091	-	-	0/4/24/31	0/1/1/1
17	HEC	Q	501	4	-	0/6/54/54	0/0/8/8
15	PEE	R	3005	-	-	0/53/53/54	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	FES	R	501	5	-	0/0/4/4	0/1/1/1

All (124) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	D	501	HEC	C3C-C2C	-11.79	1.28	1.40
17	D	501	HEC	C3B-C2B	-10.88	1.29	1.40
12	P	501	HEM	C3B-C4B	-8.44	1.44	1.51
17	Q	501	HEC	C3B-C2B	-7.93	1.32	1.40
12	C	502	HEM	C2D-C3D	-7.58	1.31	1.54
17	Q	501	HEC	C3C-C2C	-7.36	1.33	1.40
12	P	501	HEM	C3B-CAB	-7.05	1.38	1.51
12	P	502	HEM	C2D-C3D	-6.74	1.34	1.54
12	P	502	HEM	C3C-CAC	-6.62	1.38	1.51
12	P	501	HEM	C2D-C3D	-6.56	1.34	1.54
12	C	501	HEM	C3B-CAB	-6.54	1.39	1.51
12	P	502	HEM	C3B-CAB	-6.44	1.39	1.51
12	C	501	HEM	C2D-C3D	-6.20	1.35	1.54
12	C	502	HEM	C3C-CAC	-6.07	1.39	1.51
12	C	502	HEM	C3B-CAB	-6.03	1.40	1.51
12	C	501	HEM	C3B-C4B	-5.70	1.46	1.51
12	P	501	HEM	C3C-CAC	-5.70	1.40	1.51
12	P	501	HEM	C3D-C4D	-5.64	1.44	1.51
12	C	501	HEM	C3C-CAC	-5.19	1.41	1.51
12	P	501	HEM	C2C-C1C	-4.84	1.43	1.52
12	C	501	HEM	C2C-C1C	-3.48	1.46	1.52
17	D	501	HEC	C4C-NC	-3.08	1.32	1.36
12	P	502	HEM	C2C-C1C	-3.06	1.46	1.52
12	C	501	HEM	CAD-C3D	-2.92	1.48	1.54
15	E	2005	PEE	C19-C18	-2.90	1.34	1.51
15	R	3005	PEE	C19-C18	-2.87	1.34	1.51
12	P	502	HEM	C3D-C4D	-2.85	1.47	1.51
12	P	502	HEM	C3B-C4B	-2.85	1.49	1.51
12	P	501	HEM	C2D-C1D	-2.84	1.42	1.51
12	C	501	HEM	C3D-C4D	-2.84	1.47	1.51
12	P	501	HEM	C2B-C1B	-2.78	1.42	1.51
15	P	3007	PEE	C22-C21	-2.74	1.35	1.51
15	R	3005	PEE	C22-C21	-2.72	1.35	1.51
15	E	2005	PEE	C22-C21	-2.68	1.36	1.51
15	P	3007	PEE	C19-C18	-2.66	1.36	1.51
15	C	2007	PEE	C19-C18	-2.53	1.36	1.51
15	C	2007	PEE	C22-C21	-2.52	1.37	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	502	HEM	C1A-CHA	-2.26	1.33	1.39
12	P	502	HEM	C2D-C1D	-2.16	1.44	1.51
17	Q	501	HEC	C4D-CHA	-2.11	1.34	1.39
12	C	502	HEM	C4C-NC	-2.04	1.33	1.36
12	P	501	HEM	CAD-C3D	-2.03	1.50	1.54
14	P	3004	CDL	OB2-CB2	-2.00	1.36	1.44
15	E	2005	PEE	O2-C2	2.01	1.51	1.46
18	Q	3091	BOG	C1-C2	2.02	1.58	1.52
15	R	3005	PEE	O2-C2	2.02	1.51	1.46
15	P	3007	PEE	C3-C2	2.04	1.56	1.50
15	N	3008	PEE	P-O2P	2.05	1.61	1.54
14	C	2004	CDL	O1-C1	2.11	1.49	1.43
14	Q	3003	CDL	O1-C1	2.11	1.49	1.43
14	C	2004	CDL	CB3-CB4	2.12	1.56	1.50
14	P	3004	CDL	CB3-CB4	2.17	1.56	1.50
14	P	3004	CDL	O1-C1	2.20	1.50	1.43
15	C	2008	PEE	C11-C10	2.21	1.57	1.50
14	D	2003	CDL	O1-C1	2.22	1.50	1.43
15	C	2007	PEE	C3-C2	2.25	1.57	1.50
18	Q	3009	BOG	O5-C1	2.26	1.47	1.41
13	C	2002	UQ	C5-C4	2.29	1.55	1.47
15	E	2005	PEE	C11-C10	2.31	1.57	1.50
15	R	3005	PEE	C1-C2	2.36	1.57	1.50
18	D	2009	BOG	O5-C1	2.37	1.47	1.41
13	P	3002	UQ	C8-C9	2.39	1.37	1.33
13	P	3002	UQ	C5-C4	2.43	1.56	1.47
15	R	3005	PEE	C11-C10	2.45	1.58	1.50
18	D	2091	BOG	O5-C1	2.47	1.48	1.41
18	P	2010	BOG	C4-C5	2.47	1.58	1.53
13	P	3002	UQ	O2-C2	2.48	1.43	1.37
15	C	2008	PEE	C3-C2	2.48	1.57	1.50
15	R	3005	PEE	C31-C30	2.49	1.58	1.50
18	Q	3091	BOG	O5-C1	2.50	1.48	1.41
15	R	3005	PEE	C3-C2	2.52	1.57	1.50
13	C	2002	UQ	C8-C9	2.52	1.37	1.33
12	C	501	HEM	C4C-NC	2.54	1.39	1.36
18	Q	3091	BOG	C4-C5	2.55	1.58	1.53
13	P	3002	UQ	CM5-C5	2.55	1.56	1.50
15	C	2008	PEE	C1-C2	2.55	1.57	1.50
15	E	2005	PEE	C1-C2	2.56	1.57	1.50
18	P	2010	BOG	C1-C2	2.56	1.57	1.52
13	P	3002	UQ	C3-C4	2.56	1.56	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	D	2091	BOG	C4-C5	2.58	1.58	1.53
18	P	2010	BOG	O5-C1	2.60	1.48	1.43
13	C	2002	UQ	C7-C8	2.62	1.54	1.50
15	P	3007	PEE	P-O1P	2.62	1.60	1.51
13	C	2002	UQ	O2-C2	2.63	1.43	1.37
13	C	2002	UQ	CM5-C5	2.63	1.56	1.50
15	E	2005	PEE	C3-C2	2.67	1.58	1.50
13	P	3002	UQ	C7-C8	2.68	1.55	1.50
15	N	3008	PEE	P-O3P	2.74	1.64	1.54
15	C	2007	PEE	O2-C10	2.75	1.42	1.34
15	P	3007	PEE	O2-C10	2.77	1.42	1.34
13	P	3002	UQ	C2-C1	2.81	1.56	1.48
15	E	2005	PEE	C31-C30	2.83	1.59	1.50
13	C	2002	UQ	C2-C1	2.86	1.57	1.48
13	C	2002	UQ	C3-C4	2.88	1.57	1.48
15	C	2007	PEE	P-O1P	2.89	1.61	1.51
15	E	2005	PEE	P-O1P	2.96	1.62	1.51
13	P	3002	UQ	O3-C3	2.96	1.44	1.37
15	N	3008	PEE	P-O4P	2.99	1.65	1.54
15	C	2008	PEE	P-O1P	3.00	1.62	1.51
15	R	3005	PEE	P-O1P	3.06	1.62	1.51
15	C	2008	PEE	O2-C10	3.13	1.43	1.34
12	P	501	HEM	CBB-CAB	3.17	1.47	1.29
15	P	3007	PEE	O3-C30	3.18	1.42	1.33
12	C	501	HEM	CBB-CAB	3.19	1.47	1.29
13	C	2002	UQ	O3-C3	3.23	1.45	1.37
15	C	2007	PEE	O3-C30	3.25	1.43	1.33
15	R	3005	PEE	O3-C30	3.27	1.43	1.33
12	C	502	HEM	CBC-CAC	3.31	1.48	1.29
15	E	2005	PEE	O2-C10	3.35	1.44	1.34
15	C	2008	PEE	O3-C30	3.36	1.43	1.33
15	R	3005	PEE	O2-C10	3.42	1.44	1.34
13	P	3002	UQ	C6-C5	3.53	1.43	1.35
15	E	2005	PEE	O3-C30	3.54	1.44	1.33
12	C	502	HEM	CBB-CAB	3.58	1.50	1.29
13	C	2002	UQ	C6-C5	3.74	1.44	1.35
13	P	3002	UQ	C6-C1	3.78	1.57	1.46
12	P	502	HEM	CBB-CAB	3.84	1.51	1.29
12	P	502	HEM	CBC-CAC	3.92	1.51	1.29
13	C	2002	UQ	C6-C1	4.20	1.58	1.46
12	C	501	HEM	CBC-CAC	4.70	1.56	1.29
12	P	501	HEM	CBC-CAC	4.78	1.56	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	C	2002	UQ	C7-C6	5.10	1.60	1.51
13	P	3002	UQ	C7-C6	5.13	1.60	1.51
15	N	3008	PEE	P-O1P	6.24	1.62	1.50

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	D	501	HEC	CBB-CAB-C3B	-8.71	107.99	127.35
17	Q	501	HEC	CBC-CAC-C3C	-7.43	110.84	127.35
17	Q	501	HEC	CBB-CAB-C3B	-7.34	111.03	127.35
17	D	501	HEC	CBC-CAC-C3C	-6.12	113.75	127.35
12	C	501	HEM	C3B-CAB-CBB	-5.16	116.54	124.46
12	P	501	HEM	C3B-CAB-CBB	-5.08	116.66	124.46
14	P	3004	CDL	CB4-OB6-CB5	-3.68	109.06	117.89
14	C	2004	CDL	CA4-OA6-CA5	-3.51	109.47	117.89
12	C	501	HEM	CMA-C3A-C4A	-3.49	122.59	128.36
14	C	2004	CDL	CB4-OB6-CB5	-3.46	109.58	117.89
14	P	3004	CDL	CA4-OA6-CA5	-3.24	110.12	117.89
12	P	501	HEM	C3C-CAC-CBC	-3.22	119.51	124.46
12	C	501	HEM	C1D-CHD-C4C	-3.17	120.53	125.82
12	C	501	HEM	C3C-CAC-CBC	-3.05	119.78	124.46
13	P	3002	UQ	C7-C6-C1	-3.00	115.03	118.56
13	P	3002	UQ	C10-C9-C8	-2.89	117.82	123.50
13	C	2002	UQ	C7-C6-C1	-2.78	115.28	118.56
17	D	501	HEC	CAA-C2A-C3A	-2.76	121.14	129.00
13	C	2002	UQ	C10-C9-C8	-2.68	118.24	123.50
14	D	2003	CDL	CB4-OB6-CB5	-2.60	111.65	117.89
17	Q	501	HEC	CAA-C2A-C3A	-2.57	121.67	129.00
14	Q	3003	CDL	CB4-OB6-CB5	-2.56	111.75	117.89
12	P	501	HEM	CAA-C2A-C1A	-2.51	124.28	127.01
14	D	2003	CDL	CA6-CA4-CA3	-2.45	106.33	112.07
14	Q	3003	CDL	CA6-CA4-CA3	-2.36	106.56	112.07
14	P	3004	CDL	CA6-CA4-CA3	-2.26	106.78	112.07
14	Q	3003	CDL	CA4-OA6-CA5	-2.24	112.52	117.89
14	D	2003	CDL	CA6-OA8-CA7	-2.11	111.81	117.14
14	D	2003	CDL	CB6-CB4-CB3	-2.08	107.20	112.07
14	Q	3003	CDL	CA6-OA8-CA7	-2.07	111.89	117.14
14	D	2003	CDL	CA4-OA6-CA5	-2.06	112.95	117.89
14	Q	3003	CDL	CB6-CB4-CB3	-2.05	107.28	112.07
14	C	2004	CDL	CA6-CA4-CA3	-2.03	107.33	112.07
13	P	3002	UQ	C11-C9-C8	2.01	125.22	120.74
12	C	501	HEM	C2C-C1C-NC	2.01	113.60	110.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	C	2004	CDL	OB6-CB4-CB3	2.07	115.65	108.36
15	C	2007	PEE	O3-C3-C2	2.09	114.32	108.69
12	P	502	HEM	C2D-C3D-C4D	2.14	105.13	101.50
18	D	2091	BOG	O1-C1-C2	2.23	110.84	108.21
15	E	2005	PEE	O3-C3-C2	2.23	114.70	108.69
13	C	2002	UQ	C11-C9-C8	2.27	125.80	120.74
15	R	3005	PEE	C23-C22-C21	2.30	126.39	114.53
15	R	3005	PEE	O3-C3-C2	2.35	115.01	108.69
14	P	3004	CDL	OB6-CB4-CB3	2.39	116.77	108.36
15	P	3007	PEE	C22-C21-C20	2.44	127.13	114.53
15	R	3005	PEE	C19-C18-C17	2.45	127.18	114.53
15	E	2005	PEE	C23-C22-C21	2.45	127.19	114.53
18	Q	3091	BOG	O1-C1-C2	2.47	111.12	108.21
15	E	2005	PEE	C19-C18-C17	2.47	127.28	114.53
12	C	501	HEM	CMA-C3A-C2A	2.49	130.43	125.24
15	R	3005	PEE	C22-C21-C20	2.50	127.43	114.53
15	P	3007	PEE	C23-C22-C21	2.51	127.48	114.53
12	P	502	HEM	CMD-C2D-C3D	2.52	125.51	114.35
15	E	2005	PEE	C22-C21-C20	2.54	127.66	114.53
12	C	502	HEM	C1D-CHD-C4C	2.58	130.13	125.82
15	C	2007	PEE	C22-C21-C20	2.58	127.86	114.53
15	P	3007	PEE	C19-C18-C17	2.59	127.90	114.53
15	C	2007	PEE	C19-C18-C17	2.59	127.92	114.53
15	C	2007	PEE	C23-C22-C21	2.59	127.93	114.53
15	E	2005	PEE	C20-C19-C18	2.63	128.12	114.53
12	P	501	HEM	CMD-C2D-C3D	2.69	126.23	114.35
12	P	502	HEM	C3C-CAC-CBC	2.75	128.67	124.46
15	R	3005	PEE	C20-C19-C18	2.76	128.76	114.53
12	P	502	HEM	CBA-CAA-C2A	2.79	117.53	112.53
12	C	501	HEM	CAD-C3D-C2D	2.79	121.23	113.22
15	P	3007	PEE	C20-C19-C18	2.80	128.97	114.53
15	C	2007	PEE	C20-C19-C18	2.83	129.12	114.53
12	C	502	HEM	CAD-C3D-C2D	2.89	121.54	113.22
12	P	502	HEM	CAD-C3D-C2D	2.97	121.75	113.22
12	C	502	HEM	C3C-CAC-CBC	3.06	129.15	124.46
12	C	502	HEM	CMC-C2C-C3C	3.15	124.39	116.53
12	C	501	HEM	CMD-C2D-C3D	3.16	128.31	114.35
12	P	501	HEM	C2D-C3D-C4D	3.17	106.87	101.50
18	Q	3091	BOG	C1'-O1-C1	3.19	118.50	113.29
17	D	501	HEC	CBA-CAA-C2A	3.29	118.42	112.53
12	P	501	HEM	CAD-C3D-C2D	3.40	122.99	113.22
18	D	2009	BOG	C1'-O1-C1	3.54	120.13	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	Q	3009	BOG	C1'-O1-C1	3.59	120.22	113.94
12	C	501	HEM	C2D-C3D-C4D	3.60	107.61	101.50
13	P	3002	UQ	C8-C7-C6	3.70	122.76	111.64
12	P	502	HEM	CMB-C2B-C3B	3.71	125.78	116.53
12	P	501	HEM	CMB-C2B-C3B	3.71	125.79	116.53
13	C	2002	UQ	C8-C7-C6	3.74	122.88	111.64
12	C	501	HEM	CMB-C2B-C3B	3.79	125.99	116.53
17	D	501	HEC	CAD-C3D-C4D	3.82	131.16	127.01
18	D	2091	BOG	C1'-O1-C1	3.83	119.56	113.29
12	P	501	HEM	CMC-C2C-C3C	3.90	126.26	116.53
12	C	501	HEM	CMC-C2C-C3C	4.06	126.67	116.53
17	Q	501	HEC	CAD-C3D-C4D	4.26	131.63	127.01
17	Q	501	HEC	CBA-CAA-C2A	4.40	120.41	112.53
12	P	502	HEM	CMC-C2C-C3C	4.53	127.84	116.53
12	C	502	HEM	CMB-C2B-C3B	4.53	127.84	116.53
12	P	501	HEM	CAD-C3D-C4D	4.85	129.57	112.47
12	C	501	HEM	CAD-C3D-C4D	5.25	130.98	112.47
12	C	502	HEM	CAD-C3D-C4D	5.81	132.97	112.47
12	P	502	HEM	CAD-C3D-C4D	5.81	132.97	112.47
17	D	501	HEC	CAA-C2A-C1A	6.32	133.87	127.01
17	Q	501	HEC	CAA-C2A-C1A	6.81	134.40	127.01

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

19 monomers are involved in 47 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	C	2002	UQ	5	0
14	C	2004	CDL	2	0
15	C	2007	PEE	2	0
12	C	501	HEM	5	0
12	C	502	HEM	1	0
14	D	2003	CDL	2	0
18	D	2009	BOG	1	0
17	D	501	HEC	3	0
15	E	2005	PEE	1	0
19	E	501	FES	2	0
18	P	2010	BOG	1	0
13	P	3002	UQ	4	0
14	P	3004	CDL	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	P	3007	PEE	2	0
12	P	501	HEM	5	0
12	P	502	HEM	3	0
14	Q	3003	CDL	3	0
17	Q	501	HEC	1	0
19	R	501	FES	2	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<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	443/446 (99%)	0.11	3 (0%) 89 82	38, 72, 106, 123	0
1	N	442/446 (99%)	0.19	4 (0%) 85 77	41, 79, 111, 121	0
2	B	421/441 (95%)	0.51	14 (3%) 50 33	59, 90, 133, 158	0
2	O	422/441 (95%)	0.27	7 (1%) 73 59	49, 86, 120, 149	0
3	C	380/380 (100%)	-0.04	1 (0%) 94 92	25, 46, 88, 131	0
3	P	379/380 (99%)	0.03	2 (0%) 91 87	34, 70, 102, 127	0
4	D	241/241 (100%)	-0.06	2 (0%) 87 79	38, 51, 105, 124	0
4	Q	241/241 (100%)	0.31	11 (4%) 36 21	55, 88, 124, 142	0
5	E	196/196 (100%)	1.74	76 (38%) 0 0	42, 150, 175, 178	125 (63%)
5	R	196/196 (100%)	0.99	40 (20%) 1 1	51, 104, 148, 162	127 (64%)
6	F	101/110 (91%)	-0.07	0 100 100	32, 53, 74, 109	0
6	S	101/110 (91%)	0.43	5 (4%) 32 17	56, 79, 121, 145	0
7	G	80/81 (98%)	0.13	1 (1%) 79 67	37, 63, 111, 120	0
7	T	79/81 (97%)	0.69	9 (11%) 7 3	54, 99, 162, 174	0
8	H	70/77 (90%)	0.09	2 (2%) 55 39	44, 73, 98, 145	0
8	U	67/77 (87%)	1.47	18 (26%) 1 0	110, 132, 150, 155	0
9	I	31/47 (65%)	1.38	7 (22%) 1 1	80, 125, 161, 162	0
9	V	31/47 (65%)	1.43	8 (25%) 1 0	81, 114, 162, 165	0
10	J	61/61 (100%)	0.17	4 (6%) 22 11	51, 66, 113, 156	0
10	W	60/61 (98%)	0.17	2 (3%) 50 33	66, 86, 130, 135	0
All	All	4042/4160 (97%)	0.34	216 (5%) 30 16	25, 77, 143, 178	252 (6%)

All (216) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	E	157	TYR	12.0
5	E	163	SER	7.2
9	V	63	ASP	7.0
5	E	85	LYS	6.9
5	E	152	ASP	6.8
5	E	171	ILE	6.8
5	E	165	TYR	6.7
5	E	173	LYS	6.4
5	E	158	CYS	6.3
8	H	9	GLU	6.2
5	E	109	GLU	6.1
5	R	112	VAL	6.0
5	E	129	LYS	6.0
5	E	117	LEU	5.9
7	T	77	TYR	5.8
5	E	174	GLY	5.8
8	U	13	LEU	5.8
5	E	124	LEU	5.7
10	J	63	GLU	5.6
3	C	380	TYR	5.5
5	E	106	ILE	5.4
5	E	84	GLY	5.3
9	I	63	ASP	5.3
5	E	156	TYR	5.3
5	E	172	ARG	5.1
8	U	37	LEU	5.1
5	E	167	ALA	4.9
5	R	81	ILE	4.8
5	R	122	HIS	4.8
2	B	19	PRO	4.7
5	E	79	SER	4.7
5	E	107	ASN	4.7
5	E	169	GLY	4.6
5	E	177	PRO	4.6
10	J	62	SER	4.6
5	E	105	GLU	4.6
9	V	56	SER	4.5
5	R	113	ASP	4.5
5	E	134	ILE	4.4
5	E	119	ASP	4.4
5	R	124	LEU	4.3
5	E	164	HIS	4.3
5	E	168	SER	4.3

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Mol	Chain	Res	Type	RSRZ
5	E	108	GLN	4.3
5	E	120	PRO	4.3
5	E	125	ASP	4.3
5	R	172	ARG	4.2
5	E	86	ASN	4.1
5	E	83	GLU	4.1
5	E	102	THR	4.1
5	R	84	GLY	4.0
2	O	19	PRO	4.0
9	I	52	ARG	4.0
5	R	102	THR	4.0
8	H	10	GLU	4.0
5	E	115	SER	3.9
8	U	12	GLU	3.9
5	E	121	GLN	3.8
1	N	216	PHE	3.7
5	R	196	GLY	3.7
5	E	190	ASP	3.7
5	E	147	ILE	3.6
5	E	130	PRO	3.6
5	E	180	LEU	3.6
5	E	98	VAL	3.6
5	R	110	ALA	3.6
8	U	78	LYS	3.5
5	E	159	PRO	3.5
5	E	187	PHE	3.5
5	E	118	ARG	3.5
10	W	62	SER	3.5
2	O	386	ALA	3.5
5	E	185	TYR	3.4
5	E	100	HIS	3.4
7	T	80	ASP	3.4
4	Q	169	LEU	3.3
7	G	2	ILE	3.3
5	R	164	HIS	3.2
5	R	169	GLY	3.2
8	U	50	THR	3.2
5	E	178	TYR	3.2
7	T	75	ALA	3.2
5	E	135	LEU	3.2
5	E	188	VAL	3.2
5	E	81	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
5	E	116	LYS	3.2
5	E	194	VAL	3.1
6	S	11	ARG	3.1
5	E	104	ALA	3.1
5	E	162	GLY	3.1
5	R	111	GLU	3.1
5	R	171	ILE	3.1
9	I	77	ARG	3.1
5	E	103	GLN	3.1
5	R	101	ARG	3.1
2	B	224	LEU	3.1
9	I	55	MET	3.0
4	Q	143	VAL	3.0
5	R	114	VAL	3.0
5	E	128	LYS	3.0
9	V	55	MET	3.0
2	B	36	ALA	2.9
1	N	376	CYS	2.9
5	E	101	ARG	2.9
5	E	148	ALA	2.9
4	D	1	GLY	2.9
8	U	44	VAL	2.9
7	T	78	GLU	2.8
5	R	119	ASP	2.8
5	R	165	TYR	2.8
4	Q	164	ILE	2.8
7	T	2	ILE	2.8
9	V	53	GLU	2.8
8	U	49	HIS	2.8
6	S	12	LEU	2.8
5	R	103	GLN	2.8
5	R	82	PRO	2.8
1	A	102	LEU	2.7
9	I	47	ARG	2.7
10	J	64	GLU	2.7
10	J	61	ALA	2.7
5	E	175	PRO	2.7
5	R	170	ARG	2.7
5	E	114	VAL	2.7
5	R	128	LYS	2.7
5	R	191	ASP	2.7
7	T	74	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	29	LEU	2.6
5	E	153	PHE	2.6
2	B	405	VAL	2.6
5	E	151	GLY	2.6
9	V	54	SER	2.6
6	S	81	VAL	2.6
5	E	146	PRO	2.6
5	R	190	ASP	2.6
9	V	57	GLY	2.6
5	E	133	VAL	2.6
5	R	168	SER	2.6
5	E	87	VAL	2.6
5	R	117	LEU	2.6
1	A	83	GLY	2.6
5	E	113	ASP	2.5
5	R	125	ASP	2.5
2	B	221	GLU	2.5
2	B	201	SER	2.5
5	E	82	PRO	2.5
8	U	46	SER	2.5
2	O	217	LYS	2.5
5	E	122	HIS	2.5
4	Q	141	VAL	2.5
5	R	188	VAL	2.5
9	V	50	LEU	2.5
2	B	393	THR	2.4
6	S	18	LYS	2.4
8	U	48	SER	2.4
8	U	33	ALA	2.4
3	P	2	ALA	2.4
5	R	121	GLN	2.4
9	V	49	LEU	2.4
4	Q	48	PHE	2.4
5	R	157	TYR	2.4
8	U	36	ARG	2.4
5	E	182	VAL	2.3
8	U	45	SER	2.3
2	B	289	SER	2.3
3	P	380	TYR	2.3
8	U	35	GLU	2.3
5	R	77	LYS	2.3
9	I	57	GLY	2.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	B	412	ASN	2.3
4	Q	167	GLU	2.3
1	A	226	ASP	2.3
2	B	402	ILE	2.3
5	R	176	ALA	2.2
5	R	127	VAL	2.2
5	E	132	TRP	2.2
10	W	63	GLU	2.2
8	U	61	PHE	2.2
2	O	34	ILE	2.2
7	T	44	GLN	2.2
4	D	170	GLU	2.2
5	E	149	ASN	2.2
5	E	127	VAL	2.2
5	R	132	TRP	2.2
2	B	31	ASN	2.2
5	E	126	ARG	2.2
8	U	63	HIS	2.2
5	E	150	SER	2.2
7	T	70	LYS	2.2
4	Q	3	LEU	2.2
8	U	47	ARG	2.1
2	O	296	TYR	2.1
5	R	187	PHE	2.1
5	E	111	GLU	2.1
4	Q	171	TYR	2.1
5	R	78	LEU	2.1
2	B	386	ALA	2.1
1	N	127	ILE	2.1
5	E	78	LEU	2.1
4	Q	5	LEU	2.1
2	O	267	ALA	2.1
9	I	53	GLU	2.1
5	R	126	ARG	2.1
6	S	23	ALA	2.1
4	Q	113	LEU	2.1
5	E	76	ILE	2.1
7	T	73	ASN	2.1
1	N	175	LYS	2.1
2	B	223	PHE	2.1
5	R	152	ASP	2.0
8	U	54	CYS	2.0

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Mol	Chain	Res	Type	RSRZ
2	O	36	ALA	2.0
4	Q	159	GLY	2.0
8	U	57	GLU	2.0
5	R	178	TYR	2.0
5	R	76	ILE	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<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
11	UNL	C	3288	1/-	0.94	0.55	8.84	84,84,84,84	0
13	UQ	P	3002	19/63	0.69	0.59	7.80	121,130,133,133	0
15	PEE	C	2008	21/51	0.67	0.47	5.44	150,154,158,159	0
18	BOG	P	2010	12/20	0.63	0.43	5.12	155,156,157,158	0
15	PEE	E	2005	50/51	0.83	0.45	4.47	72,96,104,105	0
15	PEE	R	3005	50/51	0.80	0.42	3.47	87,109,125,125	0
14	CDL	D	2003	42/100	0.86	0.39	3.45	97,106,116,117	0
13	UQ	C	2002	19/63	0.83	0.39	3.22	82,84,86,86	0
16	GOL	P	3011	6/6	0.93	0.30	3.00	86,87,88,89	0
11	UNL	A	3284	1/-	0.95	0.40	2.81	28,28,28,28	0
14	CDL	Q	3003	42/100	0.77	0.48	2.70	134,150,157,158	0
15	PEE	P	3007	49/51	0.85	0.48	2.69	65,94,110,112	0
16	GOL	C	2011	6/6	0.92	0.31	2.66	70,71,72,75	0
15	PEE	C	2007	49/51	0.91	0.36	2.41	42,65,85,87	0
18	BOG	Q	3009	20/20	0.93	0.31	1.82	82,93,95,95	0
11	UNL	P	3286	1/-	0.77	0.37	1.79	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
14	CDL	C	2004	40/100	0.93	0.33	1.62	69,86,100,102	0
11	UNL	N	3291	1/-	0.96	0.33	1.58	37,37,37,37	0
12	HEM	P	501	43/43	0.98	0.27	1.42	48,52,61,66	0
18	BOG	D	2009	20/20	0.93	0.25	1.36	52,70,74,76	0
12	HEM	C	502	43/43	0.98	0.29	1.34	23,30,38,44	0
12	HEM	C	501	43/43	0.98	0.26	1.09	30,36,47,53	0
14	CDL	P	3004	40/100	0.87	0.39	0.98	107,115,122,124	0
12	HEM	P	502	43/43	0.98	0.27	0.50	43,50,60,65	0
17	HEC	D	501	43/43	0.99	0.22	-0.15	35,40,48,52	0
17	HEC	Q	501	43/43	0.97	0.25	-0.34	70,75,81,84	0
19	FES	E	501	4/4	0.94	0.13	-1.55	161,162,162,162	4
19	FES	R	501	4/4	0.98	0.09	-2.11	92,94,94,95	4
11	UNL	N	3290	1/-	0.80	0.47	-	53,53,53,53	0
11	UNL	N	4231	1/-	0.81	0.55	-	67,67,67,67	0
11	UNL	A	3289	1/-	0.88	0.69	-	38,38,38,38	0
18	BOG	Q	3091	13/20	0.47	0.60	-	195,196,196,196	0
18	BOG	D	2091	13/20	0.33	0.84	-	185,187,187,187	0
11	UNL	A	3231	1/-	0.52	0.65	-	91,91,91,91	0
15	PEE	N	3008	5/51	0.72	0.28	-	117,118,119,119	0
11	UNL	C	3287	1/-	0.86	0.95	-	88,88,88,88	0

## 6.5 Other polymers

There are no such residues in this entry.