



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 13, 2024 – 09:59 am BST

PDB ID : 1QLE  
Title : CRYO-STRUCTURE OF THE PARACOCCLUS DENITRIFICANS FOUR-SUBUNIT CYTOCHROME C OXIDASE IN THE COMPLETELY OXIDIZED STATE COMPLEXED WITH AN ANTIBODY FV FRAGMENT  
Authors : Harrenga, A.; Michel, H.  
Deposited on : 1999-08-30  
Resolution : 3.00 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

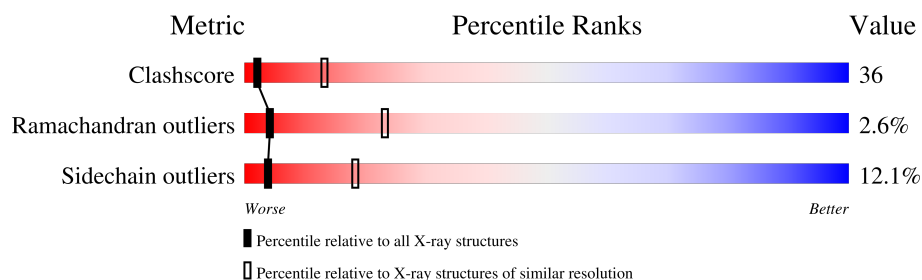
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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))
Clashscore	180529	2866 (3.00-3.00)
Ramachandran outliers	177936	2778 (3.00-3.00)
Sidechain outliers	177891	2781 (3.00-3.00)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	538	<div> <div>35%</div> <div>56%</div> <div>8%</div> </div>
2	B	252	<div> <div>46%</div> <div>46%</div> <div>8%</div> </div>
3	C	273	<div> <div>45%</div> <div>48%</div> <div>8%</div> </div>
4	D	43	<div> <div>63%</div> <div>33%</div> <div>5%</div> </div>
5	H	119	<div> <div>31%</div> <div>64%</div> <div>5%</div> </div>
6	L	108	<div> <div>41%</div> <div>50%</div> <div>9%</div> </div>

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 10762 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 CYTOCHROME C OXIDASE POLYPEPTIDE I-BETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	538	Total	C	N	O	S	0	0	0
			4269	2860	671	705	33			

- Molecule 2 is a protein called CYTOCHROME C OXIDASE POLYPEPTIDE II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	252	Total	C	N	O	S	0	0	0
			1977	1295	319	355	8			

- Molecule 3 is a protein called CYTOCHROME C OXIDASE POLYPEPTIDE III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	273	Total	C	N	O	S	0	0	0
			2181	1483	339	348	11			

- Molecule 4 is a protein called CCYTOCHROME C OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	43	Total	C	N	O	S	0	0	0
			332	214	58	59	1			

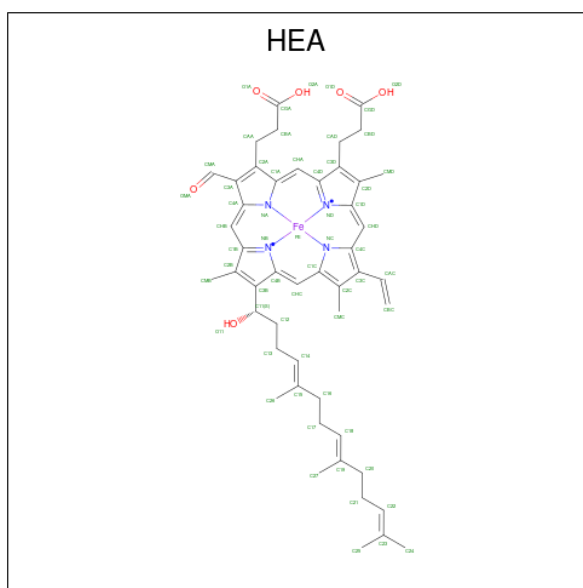
- Molecule 5 is a protein called HEAVY CHAIN ANTIBODY FV FRAGMENT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	H	119	Total	C	N	O	S	0	0	0
			938	589	157	186	6			

- Molecule 6 is a protein called LIGHT CHAIN ANTIBODY FV FRAGMENT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	L	108	Total	C	N	O	S	0	0	0
			832	530	135	165	2			

- Molecule 7 is HEME-A (three-letter code: HEA) (formula:  $C_{49}H_{56}FeN_4O_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	Fe	N	O	
			60	49	1	4	6	0
7	A	1	Total	C	Fe	N	O	
			60	49	1	4	6	0

- Molecule 8 is COPPER (II) ION (three-letter code: CU) (formula:  $Cu$ ).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Cu		
			1	1	0	0

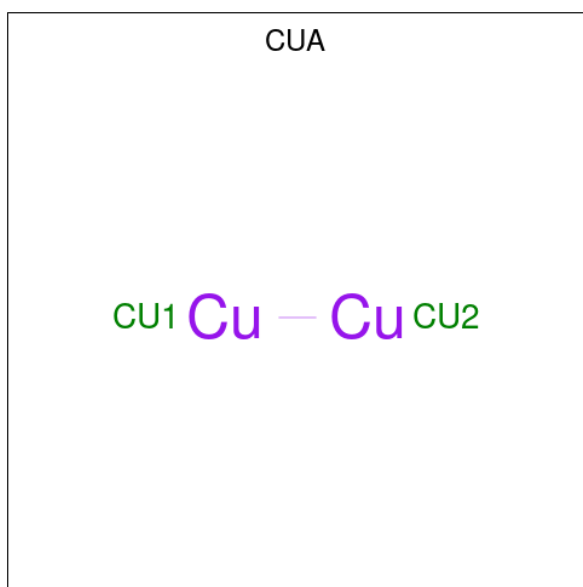
- Molecule 9 is CALCIUM ION (three-letter code: CA) (formula:  $Ca$ ).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	Ca		
			1	1	0	0

- Molecule 10 is MANGANESE (II) ION (three-letter code: MN) (formula:  $Mn$ ).

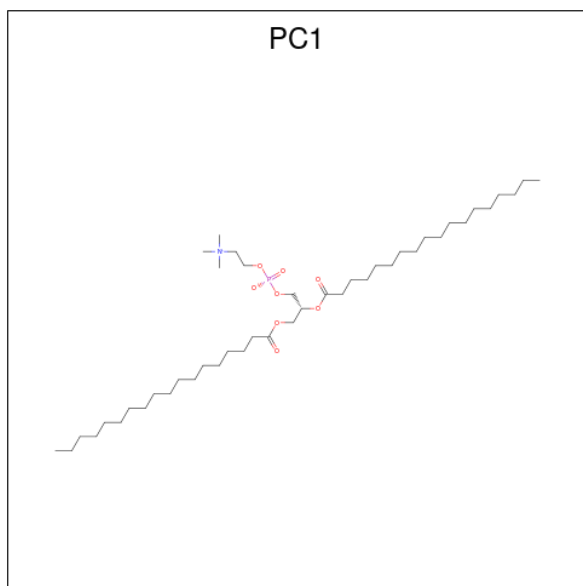
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	1	Total	Mn		
			1	1	0	0

- Molecule 11 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula:  $Cu_2$ ).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	B	1	Total	Cu	0	0
			2	2		

- Molecule 12 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula:  $C_{44}H_{88}NO_8P$ ).



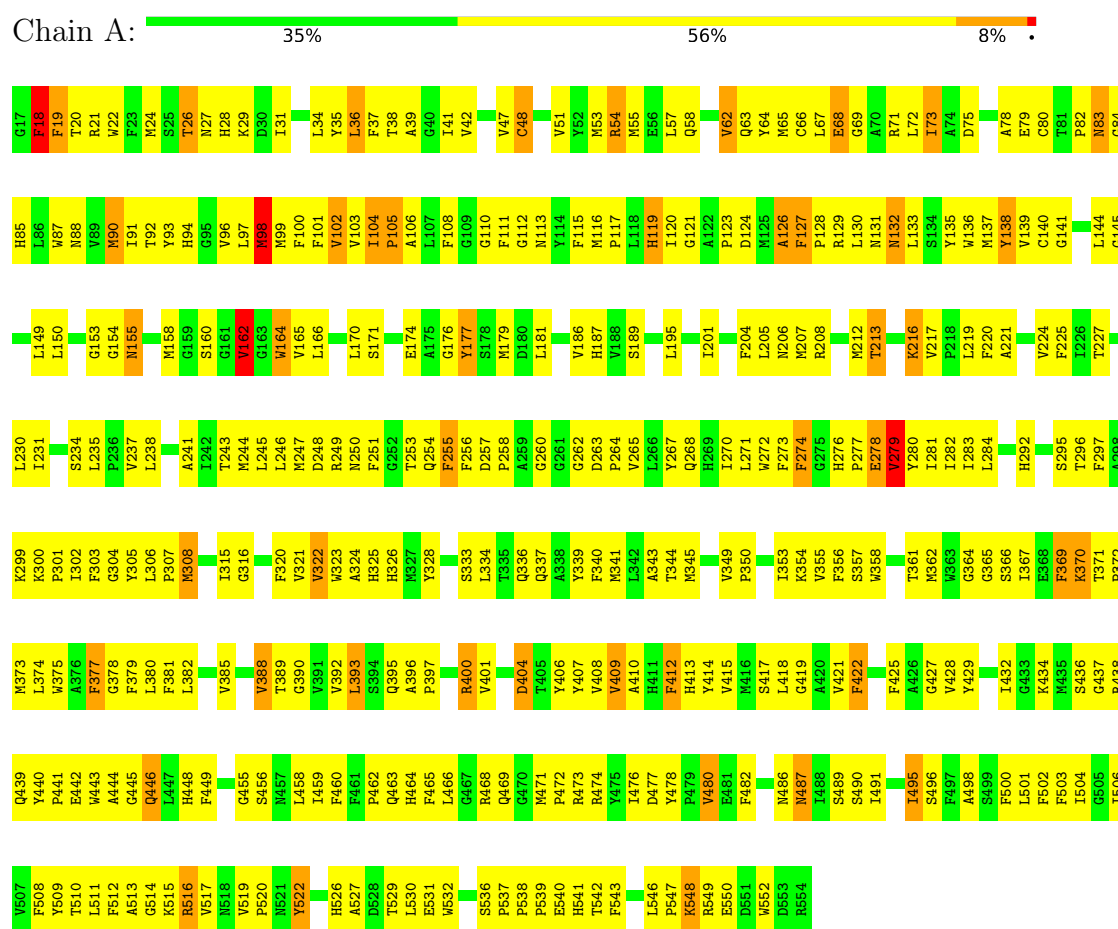
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	C	1	Total	C	N	O	P	0	0
			54	44	1	8	1		
12	C	1	Total	C	N	O	P	0	0
			54	44	1	8	1		

### 3 Residue-property plots

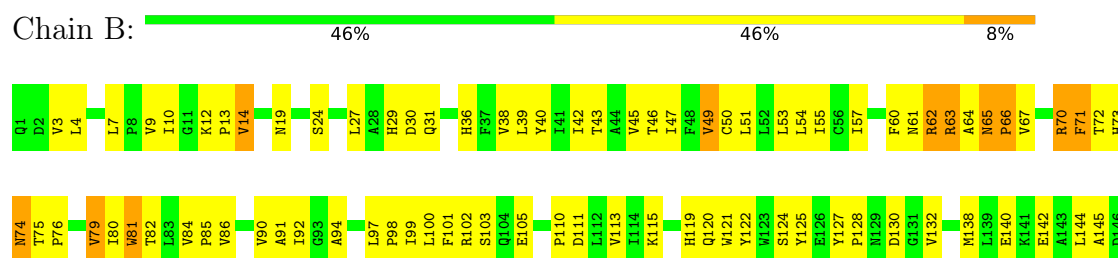
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

#### • Molecule 1: CYTOCHROME C OXIDASE POLYPEPTIDE I-BETA



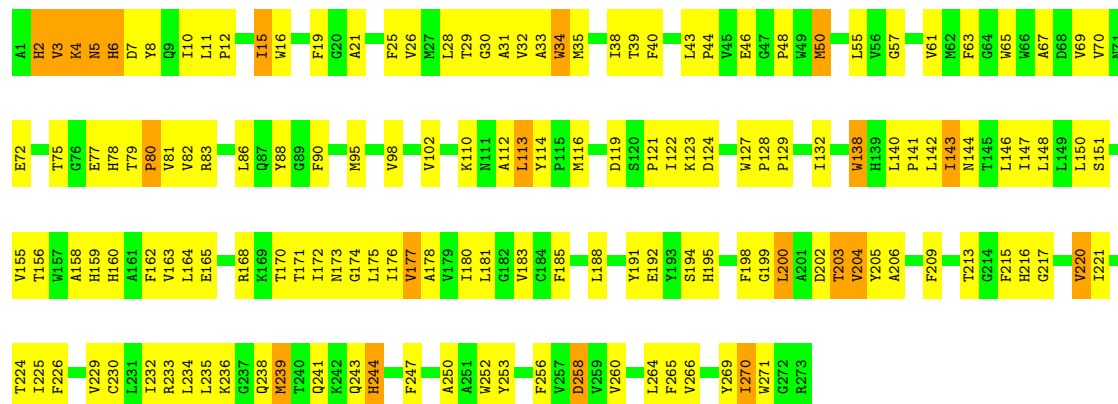
#### • Molecule 2: CYTOCHROME C OXIDASE POLYPEPTIDE II





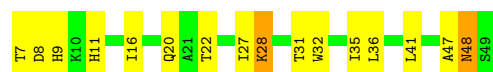
• Molecule 3: CYTOCHROME C OXIDASE POLYPEPTIDE III

Chain C: 45% 48% 8%



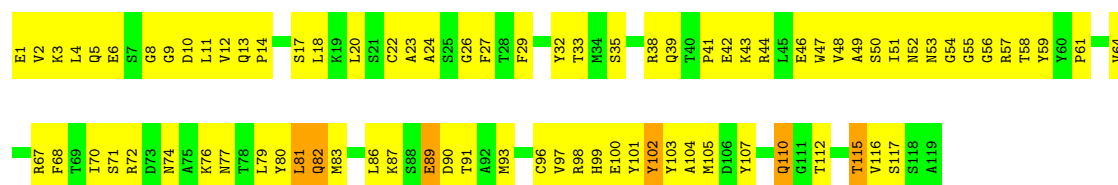
• Molecule 4: CCYTOCHROME C OXIDASE

Chain D: 63% 33% 5%



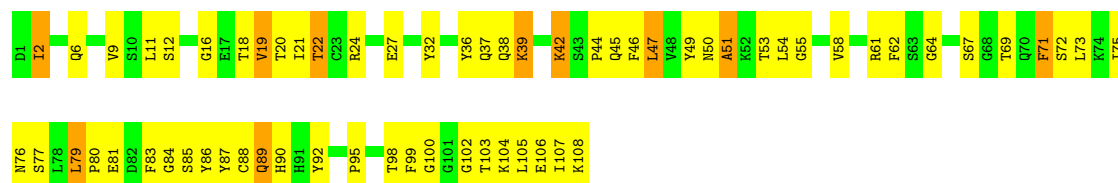
• Molecule 5: HEAVY CHAIN ANTIBODY FV FRAGMENT

Chain H: 31% 64% 5%



• Molecule 6: LIGHT CHAIN ANTIBODY FV FRAGMENT

Chain L: 41% 50% 9%



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 4	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	205.20Å 205.20Å 81.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 3.00	Depositor
% Data completeness (in resolution range)	66.2 (6.00-3.00)	Depositor
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 0.3	Depositor
R, $R_{free}$	0.235 , 0.309	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10762	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP



## 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: MN, CU, CUA, CA, HEA, PC1

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	0.59	0/4428	0.74	3/6042 (0.0%)
2	B	0.56	0/2034	0.75	0/2787
3	C	0.56	1/2267 (0.0%)	0.70	1/3103 (0.0%)
4	D	0.49	0/339	0.66	1/457 (0.2%)
5	H	0.59	0/960	0.73	0/1298
6	L	0.53	0/853	0.74	0/1156
All	All	0.57	1/10881 (0.0%)	0.73	5/14843 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	252	TRP	CB-CG	6.38	1.61	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	516	ARG	NE-CZ-NH2	7.20	123.90	120.30
3	C	35	MET	CG-SD-CE	6.13	110.01	100.20
1	A	98	MET	CG-SD-CE	6.00	109.80	100.20
1	A	99	MET	CG-SD-CE	5.90	109.65	100.20
4	D	36	LEU	CA-CB-CG	5.12	127.07	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4269	0	4184	366	0
2	B	1977	0	1963	148	0
3	C	2181	0	2151	178	0
4	D	332	0	331	12	0
5	H	938	0	894	72	0
6	L	832	0	807	54	0
7	A	120	0	108	32	0
8	A	1	0	0	0	0
9	A	1	0	0	0	0
10	A	1	0	0	0	0
11	B	2	0	0	0	0
12	C	108	0	176	26	0
All	All	10762	0	10614	778	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 36.

All (778) 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:B:4:LEU:HD11	2:B:242:TRP:CD1	1.25	1.68
2:B:4:LEU:CD1	2:B:242:TRP:CD1	2.15	1.27
3:C:2:HIS:O	3:C:3:VAL:HG22	1.13	1.25
5:H:6:GLU:OE1	5:H:96:CYS:N	1.66	1.25
2:B:159:ASP:O	2:B:161:PRO:HD3	1.37	1.22
3:C:6:HIS:HE1	3:C:8:TYR:O	1.30	1.12
5:H:6:GLU:OE1	5:H:96:CYS:SG	2.08	1.11
2:B:72:THR:HG23	2:B:73:HIS:ND1	1.66	1.09
3:C:2:HIS:O	3:C:3:VAL:CG2	2.02	1.06
3:C:6:HIS:CE1	3:C:8:TYR:O	2.10	1.04
1:A:98:MET:SD	7:A:601:HEA:C2C	2.48	1.01
1:A:365:GLY:HA2	2:B:60:PHE:HB3	1.42	1.01
2:B:190:VAL:HG11	2:B:202:LEU:HD13	1.41	1.01
2:B:138:MET:HE3	2:B:155:LEU:HA	1.40	1.01
2:B:180:ILE:HG22	2:B:218:GLU:HG2	1.45	0.98
3:C:4:LYS:NZ	4:D:7:THR:OG1	2.03	0.92
2:B:159:ASP:O	2:B:161:PRO:CD	2.18	0.92
1:A:162:VAL:HG12	1:A:170:LEU:HG	1.52	0.92
3:C:129:PRO:HG2	3:C:203:THR:HG21	1.51	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4:LEU:CD1	2:B:242:TRP:HD1	1.65	0.91
1:A:205:LEU:HA	1:A:208:ARG:NH1	1.86	0.90
1:A:205:LEU:HA	1:A:208:ARG:HH12	1.37	0.89
1:A:129:ARG:HE	3:C:65:TRP:HE1	1.15	0.88
3:C:6:HIS:ND1	3:C:6:HIS:C	2.27	0.87
5:H:6:GLU:OE1	5:H:96:CYS:CB	2.21	0.87
1:A:276:HIS:NE2	1:A:280:TYR:CE2	2.45	0.85
2:B:72:THR:HG23	2:B:73:HIS:CE1	2.12	0.84
5:H:6:GLU:OE1	5:H:96:CYS:CA	2.25	0.83
3:C:6:HIS:HE2	3:C:10:ILE:HD11	1.43	0.83
6:L:39:LYS:HB3	6:L:42:LYS:HB2	1.61	0.83
1:A:434:LYS:NZ	1:A:536:SER:HB3	1.94	0.82
2:B:86:VAL:O	2:B:90:VAL:HG23	1.79	0.82
1:A:502:PHE:CE2	1:A:506:ILE:HD11	2.15	0.81
1:A:476:ILE:HG23	1:A:477:ASP:H	1.44	0.81
2:B:4:LEU:HD11	2:B:242:TRP:HD1	1.02	0.81
2:B:4:LEU:O	2:B:7:LEU:HG	1.81	0.80
5:H:71:SER:HB3	5:H:80:TYR:HB2	1.61	0.80
1:A:83:ASN:H	1:A:83:ASN:HD22	1.27	0.80
3:C:243:GLN:HB3	12:C:302:PC1:H143	1.65	0.79
5:H:72:ARG:HH11	5:H:72:ARG:HG2	1.47	0.79
1:A:100:PHE:CE1	1:A:186:VAL:HG13	2.18	0.78
3:C:209:PHE:HE1	3:C:269:TYR:HE1	1.31	0.78
2:B:4:LEU:HD11	2:B:242:TRP:NE1	1.95	0.78
1:A:165:VAL:HB	1:A:271:LEU:HD21	1.65	0.78
2:B:162:VAL:HG13	2:B:231:VAL:HG23	1.64	0.78
5:H:5:GLN:O	5:H:22:CYS:HA	1.84	0.78
5:H:67:ARG:HH12	5:H:87:LYS:HE3	1.46	0.78
1:A:153:GLY:HA2	1:A:176:GLY:HA3	1.65	0.78
1:A:267:TYR:CE2	1:A:271:LEU:HD22	2.19	0.78
3:C:4:LYS:HZ3	4:D:7:THR:HA	1.49	0.78
5:H:2:VAL:HG13	5:H:27:PHE:CD1	2.19	0.78
3:C:6:HIS:ND1	3:C:7:ASP:N	2.32	0.77
3:C:65:TRP:O	3:C:69:VAL:HG23	1.84	0.77
1:A:365:GLY:HA3	2:B:65:ASN:HD22	1.48	0.77
1:A:83:ASN:HD22	1:A:83:ASN:N	1.82	0.77
2:B:198:ARG:HB2	3:C:121:PRO:HD3	1.68	0.75
1:A:98:MET:SD	7:A:601:HEA:C3C	2.75	0.75
1:A:279:VAL:HB	7:A:602:HEA:HAC	1.67	0.75
3:C:80:PRO:HA	3:C:83:ARG:HG3	1.69	0.75
6:L:79:LEU:HB3	6:L:81:GLU:OE2	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4:LEU:HD22	2:B:234:VAL:HG11	1.67	0.74
3:C:127:TRP:HB3	3:C:128:PRO:HD3	1.68	0.74
1:A:276:HIS:NE2	1:A:280:TYR:HE2	1.84	0.74
2:B:12:LYS:HD2	2:B:213:PHE:HE1	1.53	0.74
1:A:201:ILE:HG23	1:A:225:PHE:HE1	1.51	0.73
1:A:88:ASN:O	1:A:91:ILE:HG13	1.88	0.73
1:A:324:ALA:HB3	1:A:340:PHE:CG	2.24	0.73
1:A:412:PHE:CE1	1:A:413:HIS:CE1	2.77	0.73
6:L:87:TYR:CE2	6:L:102:GLY:HA3	2.23	0.73
1:A:367:ILE:H	2:B:61:ASN:HA	1.51	0.73
3:C:4:LYS:O	3:C:4:LYS:HG3	1.86	0.73
1:A:47:VAL:HG21	7:A:601:HEA:H171	1.69	0.73
1:A:55:MET:HB3	1:A:64:TYR:CE2	2.23	0.73
3:C:148:LEU:HB3	3:C:258:ASP:OD2	1.89	0.73
5:H:38:ARG:HH12	5:H:90:ASP:HA	1.54	0.73
1:A:434:LYS:HZ3	1:A:536:SER:HB3	1.54	0.72
3:C:225:ILE:HG21	12:C:302:PC1:H3A2	1.71	0.72
1:A:414:TYR:HE1	1:A:460:PHE:HB2	1.54	0.72
3:C:162:PHE:HB2	3:C:171:THR:OG1	1.89	0.72
1:A:428:VAL:O	1:A:432:ILE:HB	1.89	0.71
1:A:115:PHE:HB3	1:A:119:HIS:CE1	2.24	0.71
1:A:201:ILE:HG23	1:A:225:PHE:CE1	2.25	0.71
1:A:160:SER:OG	1:A:179:MET:HG2	1.91	0.71
5:H:6:GLU:CD	5:H:96:CYS:SG	2.68	0.71
6:L:21:ILE:HG13	6:L:73:LEU:HB3	1.73	0.71
3:C:138:TRP:CZ3	3:C:270:ILE:HD11	2.26	0.71
5:H:2:VAL:HB	5:H:107:TYR:CE1	2.26	0.71
3:C:216:HIS:HD2	3:C:260:VAL:HG12	1.56	0.70
6:L:107:ILE:HD12	6:L:107:ILE:H	1.57	0.70
3:C:127:TRP:O	3:C:129:PRO:HD3	1.92	0.69
5:H:51:ILE:HG13	5:H:58:THR:HG22	1.74	0.69
1:A:366:SER:H	2:B:65:ASN:HB3	1.56	0.69
3:C:180:ILE:O	3:C:183:VAL:HG12	1.92	0.69
3:C:162:PHE:O	3:C:241:GLN:HG2	1.91	0.69
3:C:168:ARG:HH22	3:C:239:MET:H	1.37	0.69
6:L:2:ILE:HG21	6:L:27:GLU:HG2	1.75	0.69
2:B:243:LEU:HD22	2:B:247:LYS:HZ1	1.58	0.69
3:C:129:PRO:CG	3:C:203:THR:HG21	2.23	0.69
1:A:38:THR:O	1:A:42:VAL:HG23	1.93	0.69
1:A:133:LEU:O	1:A:137:MET:HG2	1.93	0.69
7:A:602:HEA:H22	2:B:45:VAL:HG11	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:159:HIS:O	3:C:163:VAL:HG23	1.92	0.69
1:A:410:ALA:HB2	1:A:463:GLN:HB2	1.74	0.68
2:B:247:LYS:HB2	2:B:247:LYS:NZ	2.07	0.68
6:L:9:VAL:O	6:L:103:THR:HA	1.93	0.68
3:C:43:LEU:HB2	3:C:44:PRO:HD2	1.75	0.68
3:C:266:VAL:O	3:C:270:ILE:HB	1.94	0.68
6:L:83:PHE:CE2	6:L:107:ILE:HA	2.28	0.68
1:A:365:GLY:HA3	2:B:65:ASN:ND2	2.07	0.68
2:B:101:PHE:O	2:B:105:GLU:HB2	1.92	0.68
1:A:104:ILE:HD11	1:A:282:ILE:HA	1.76	0.68
5:H:2:VAL:HG13	5:H:27:PHE:HD1	1.57	0.68
5:H:91:THR:HG22	5:H:116:VAL:H	1.58	0.68
1:A:414:TYR:CE1	1:A:460:PHE:HB2	2.29	0.68
2:B:49:VAL:O	2:B:53:LEU:HB2	1.93	0.68
2:B:115:LYS:HG3	2:B:173:GLN:HG3	1.75	0.67
5:H:22:CYS:HB3	5:H:79:LEU:HB3	1.74	0.67
1:A:27:ASN:O	1:A:31:ILE:HG13	1.94	0.67
1:A:529:THR:HB	1:A:531:GLU:HG2	1.76	0.67
1:A:238:LEU:HD22	1:A:274:PHE:CZ	2.30	0.67
3:C:233:ARG:NH2	12:C:302:PC1:O12	2.28	0.67
1:A:238:LEU:HD22	1:A:274:PHE:CE1	2.29	0.67
6:L:18:THR:HG23	6:L:76:ASN:HA	1.76	0.67
2:B:12:LYS:HD2	2:B:213:PHE:CE1	2.29	0.67
2:B:51:LEU:O	2:B:55:ILE:HG13	1.94	0.67
2:B:165:PRO:HD3	2:B:239:TYR:CE2	2.30	0.67
3:C:88:TYR:OH	4:D:22:THR:HG22	1.94	0.67
2:B:10:ILE:HD11	2:B:210:GLY:HA3	1.76	0.67
1:A:100:PHE:HE1	1:A:186:VAL:HG13	1.60	0.66
1:A:111:PHE:O	1:A:220:PHE:HZ	1.77	0.66
1:A:296:THR:HA	1:A:526:HIS:O	1.96	0.66
5:H:13:GLN:HA	5:H:117:SER:O	1.95	0.66
1:A:98:MET:SD	7:A:601:HEA:CMC	2.84	0.66
3:C:173:ASN:HA	3:C:176:ILE:HD12	1.78	0.66
1:A:328:TYR:OH	1:A:341:MET:HA	1.96	0.66
3:C:4:LYS:NZ	4:D:7:THR:HA	2.10	0.65
3:C:119:ASP:HB3	3:C:123:LYS:HB2	1.76	0.65
5:H:32:TYR:O	5:H:53:ASN:HB3	1.95	0.65
1:A:356:PHE:HD1	2:B:81:TRP:HB2	1.61	0.65
3:C:112:ALA:HA	3:C:127:TRP:CD2	2.31	0.65
1:A:500:PHE:O	1:A:504:ILE:HG13	1.97	0.65
1:A:466:LEU:HD22	1:A:471:MET:SD	2.36	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:MET:O	1:A:103:VAL:HG23	1.97	0.65
1:A:241:ALA:HB2	1:A:270:ILE:HG22	1.79	0.64
3:C:4:LYS:O	3:C:4:LYS:CG	2.44	0.64
1:A:276:HIS:CE1	1:A:280:TYR:HE2	2.14	0.64
3:C:216:HIS:CD2	3:C:260:VAL:HG12	2.31	0.64
1:A:339:TYR:CD2	1:A:340:PHE:N	2.65	0.64
2:B:74:ASN:ND2	2:B:76:PRO:HG2	2.12	0.64
1:A:530:LEU:HG	1:A:552:TRP:HB3	1.80	0.64
2:B:243:LEU:HD22	2:B:247:LYS:NZ	2.13	0.64
1:A:437:GLY:CA	1:A:537:PRO:HD3	2.28	0.64
3:C:30:GLY:HA2	3:C:50:MET:HB3	1.79	0.64
3:C:221:ILE:O	3:C:225:ILE:HG12	1.98	0.63
5:H:1:GLU:O	5:H:26:GLY:HA3	1.98	0.63
1:A:341:MET:HG3	1:A:396:ALA:H	1.62	0.63
2:B:121:TRP:CD1	2:B:223:ASN:HB2	2.33	0.63
1:A:73:ILE:HD12	1:A:73:ILE:H	1.63	0.63
1:A:92:THR:O	1:A:96:VAL:HG23	1.99	0.63
1:A:251:PHE:HB3	3:C:200:LEU:HD23	1.81	0.63
2:B:4:LEU:HD21	2:B:242:TRP:HB2	1.80	0.63
2:B:115:LYS:HG3	2:B:173:GLN:HE21	1.63	0.63
1:A:237:VAL:HG11	1:A:273:PHE:HD1	1.62	0.63
1:A:455:GLY:HA3	1:A:495:ILE:HG12	1.81	0.63
1:A:253:THR:HG22	3:C:200:LEU:HG	1.81	0.62
1:A:476:ILE:HG23	1:A:477:ASP:N	2.14	0.62
3:C:55:LEU:HD21	12:C:302:PC1:H3H1	1.81	0.62
6:L:21:ILE:HD11	6:L:73:LEU:HD23	1.79	0.62
1:A:129:ARG:NE	3:C:65:TRP:HE1	1.94	0.62
1:A:436:SER:O	1:A:438:ARG:HD2	1.99	0.62
1:A:379:PHE:HD1	1:A:419:GLY:O	1.82	0.62
1:A:463:GLN:HA	1:A:466:LEU:HD12	1.82	0.62
2:B:209:GLU:HB2	2:B:233:ALA:O	2.00	0.62
5:H:72:ARG:HG2	5:H:72:ARG:NH1	2.15	0.62
1:A:116:MET:HB3	1:A:117:PRO:HD3	1.81	0.62
1:A:62:VAL:O	1:A:80:CYS:SG	2.58	0.62
1:A:130:LEU:HD11	1:A:195:LEU:CD2	2.29	0.62
1:A:67:LEU:HD23	1:A:67:LEU:O	1.99	0.62
1:A:120:ILE:HA	1:A:212:MET:SD	2.39	0.62
3:C:142:LEU:O	3:C:146:LEU:HG	1.99	0.62
5:H:83:MET:HB3	5:H:86:LEU:HD11	1.81	0.62
1:A:295:SER:OG	1:A:302:ILE:HG12	2.00	0.61
1:A:55:MET:HB3	1:A:64:TYR:HE2	1.63	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:160:HIS:CD2	3:C:164:LEU:HD13	2.35	0.61
1:A:530:LEU:CD2	1:A:552:TRP:HB3	2.30	0.61
1:A:31:ILE:HG12	1:A:132:ASN:HD21	1.65	0.61
1:A:401:VAL:HG21	2:B:31:GLN:NE2	2.15	0.61
1:A:179:MET:HG3	1:A:249:ARG:HH12	1.66	0.61
1:A:272:TRP:O	1:A:323:TRP:HB2	2.01	0.61
1:A:500:PHE:HB2	7:A:601:HEA:H261	1.83	0.61
3:C:158:ALA:HB1	3:C:175:LEU:HD22	1.82	0.61
1:A:382:LEU:HD13	1:A:418:LEU:HD13	1.83	0.61
5:H:14:PRO:HD3	5:H:117:SER:O	2.01	0.60
6:L:55:GLY:O	6:L:58:VAL:HG23	2.01	0.60
1:A:443:TRP:HA	1:A:446:GLN:HB2	1.83	0.60
2:B:72:THR:CG2	2:B:73:HIS:CE1	2.84	0.60
1:A:530:LEU:HD21	1:A:552:TRP:HB3	1.84	0.60
2:B:27:LEU:HD11	2:B:203:TRP:CH2	2.35	0.60
1:A:47:VAL:HG23	1:A:98:MET:CE	2.31	0.59
1:A:546:LEU:HG	3:C:5:ASN:O	2.01	0.59
6:L:2:ILE:HD11	6:L:90:HIS:ND1	2.17	0.59
1:A:530:LEU:CG	1:A:552:TRP:HB3	2.32	0.59
3:C:81:VAL:HG23	3:C:82:VAL:N	2.17	0.59
1:A:246:LEU:HG	1:A:250:ASN:HD22	1.67	0.59
5:H:105:MET:SD	6:L:99:PHE:HZ	2.26	0.59
6:L:84:GLY:O	6:L:105:LEU:N	2.33	0.59
1:A:441:PRO:HA	1:A:515:LYS:NZ	2.17	0.59
3:C:6:HIS:HE1	3:C:8:TYR:C	2.04	0.59
1:A:64:TYR:O	1:A:66:CYS:SG	2.60	0.59
1:A:71:ARG:HE	1:A:75:ASP:CG	2.06	0.59
1:A:502:PHE:CD2	1:A:506:ILE:HD11	2.36	0.59
1:A:130:LEU:HD11	1:A:195:LEU:HD22	1.83	0.59
1:A:230:LEU:HD23	1:A:320:PHE:HE1	1.67	0.59
1:A:548:LYS:HD3	1:A:550:GLU:H	1.67	0.59
1:A:230:LEU:HD23	1:A:320:PHE:CE1	2.38	0.59
2:B:46:THR:O	2:B:49:VAL:HG12	2.03	0.59
1:A:434:LYS:HZ1	1:A:536:SER:HB3	1.68	0.58
2:B:211:VAL:HG22	2:B:232:LYS:HG2	1.84	0.58
1:A:98:MET:HB3	7:A:601:HEA:HAC	1.84	0.58
3:C:170:THR:HA	3:C:173:ASN:OD1	2.04	0.58
5:H:20:LEU:HD12	5:H:81:LEU:HD12	1.85	0.58
2:B:84:VAL:HB	2:B:85:PRO:HD3	1.85	0.58
2:B:119:HIS:HB2	2:B:122:TYR:O	2.03	0.58
5:H:33:THR:O	5:H:99:HIS:HB2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:LEU:HD11	3:C:29:THR:HG22	1.86	0.58
2:B:188:PHE:CE2	2:B:231:VAL:HG11	2.39	0.58
3:C:39:THR:HA	3:C:44:PRO:HA	1.86	0.58
1:A:66:CYS:HB3	1:A:80:CYS:HA	1.86	0.57
1:A:412:PHE:HA	1:A:415:VAL:HG22	1.85	0.57
1:A:429:TYR:CE2	1:A:503:PHE:HE1	2.23	0.57
2:B:172:VAL:HB	2:B:202:LEU:HD11	1.87	0.57
1:A:299:LYS:NZ	1:A:366:SER:HB2	2.20	0.57
5:H:11:LEU:HD13	5:H:115:THR:HB	1.87	0.57
1:A:63:GLN:O	1:A:66:CYS:SG	2.63	0.57
1:A:362:MET:SD	1:A:377:PHE:CE2	2.98	0.57
1:A:371:THR:HG21	1:A:429:TYR:HD1	1.69	0.57
5:H:3:LYS:O	5:H:24:ALA:HA	2.05	0.57
1:A:31:ILE:HG12	1:A:132:ASN:ND2	2.20	0.57
1:A:217:VAL:HG12	1:A:221:ALA:HB3	1.87	0.57
1:A:397:PRO:HD3	2:B:100:LEU:HB2	1.87	0.57
2:B:172:VAL:HB	2:B:202:LEU:CD1	2.35	0.57
3:C:34:TRP:NE1	3:C:48:PRO:HG3	2.20	0.57
3:C:57:GLY:O	3:C:61:VAL:HG23	2.05	0.57
6:L:81:GLU:H	6:L:81:GLU:CD	2.09	0.57
1:A:75:ASP:HB2	1:A:78:ALA:HB3	1.86	0.57
2:B:10:ILE:CD1	2:B:210:GLY:HA3	2.35	0.57
3:C:2:HIS:C	3:C:3:VAL:HG22	2.15	0.57
1:A:129:ARG:HB2	3:C:65:TRP:CZ2	2.40	0.56
1:A:548:LYS:HD3	1:A:549:ARG:N	2.20	0.56
5:H:97:VAL:HG21	5:H:105:MET:HG2	1.87	0.56
6:L:38:GLN:HE21	6:L:44:PRO:HD3	1.70	0.56
1:A:65:MET:HB3	1:A:83:ASN:HD21	1.70	0.56
1:A:171:SER:HB3	1:A:179:MET:HE2	1.87	0.56
2:B:160:ASN:N	2:B:160:ASN:HD22	2.03	0.56
3:C:69:VAL:HG12	12:C:302:PC1:H32	1.88	0.56
1:A:73:ILE:HD12	1:A:73:ILE:N	2.20	0.56
3:C:209:PHE:CE1	3:C:269:TYR:HE1	2.17	0.56
1:A:220:PHE:O	1:A:224:VAL:HG23	2.05	0.56
1:A:409:VAL:HG12	1:A:409:VAL:O	2.06	0.56
7:A:602:HEA:H261	7:A:602:HEA:H273	1.88	0.56
1:A:268:GLN:O	1:A:272:TRP:HB2	2.06	0.56
1:A:303:PHE:CZ	2:B:73:HIS:HA	2.41	0.56
1:A:300:LYS:HD3	1:A:364:GLY:HA3	1.87	0.55
1:A:388:VAL:HG13	2:B:42:ILE:HB	1.88	0.55
1:A:429:TYR:HE2	1:A:503:PHE:HE1	1.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:76:PRO:O	2:B:79:VAL:HG12	2.06	0.55
1:A:395:GLN:OE1	2:B:92:ILE:HG22	2.06	0.55
2:B:165:PRO:HD3	2:B:239:TYR:CD2	2.41	0.55
3:C:43:LEU:HD23	3:C:43:LEU:H	1.68	0.55
3:C:146:LEU:O	3:C:150:LEU:HB2	2.06	0.55
6:L:20:THR:HA	6:L:73:LEU:O	2.06	0.55
1:A:20:THR:HA	1:A:24:MET:SD	2.46	0.55
1:A:245:LEU:HD23	1:A:256:PHE:HE1	1.71	0.55
1:A:321:VAL:HG12	12:C:301:PC1:H3E1	1.89	0.55
3:C:63:PHE:O	3:C:67:ALA:HB2	2.07	0.55
3:C:175:LEU:HD21	3:C:247:PHE:CZ	2.40	0.55
6:L:46:PHE:HZ	6:L:49:TYR:HB3	1.71	0.55
1:A:28:HIS:NE2	1:A:29:LYS:HG3	2.21	0.55
3:C:199:GLY:O	3:C:206:ALA:HB1	2.06	0.55
1:A:98:MET:HB3	7:A:601:HEA:CAC	2.36	0.55
3:C:95:MET:O	3:C:98:VAL:HB	2.06	0.55
5:H:100:GLU:O	5:H:104:ALA:HB3	2.06	0.55
1:A:280:TYR:O	1:A:284:LEU:HD23	2.07	0.55
1:A:367:ILE:HG23	1:A:373:MET:HE2	1.89	0.55
1:A:495:ILE:O	1:A:498:ALA:HB3	2.06	0.54
1:A:83:ASN:N	1:A:83:ASN:ND2	2.54	0.54
1:A:355:VAL:HA	1:A:358:TRP:HE3	1.71	0.54
1:A:421:VAL:HG21	7:A:601:HEA:H273	1.88	0.54
1:A:254:GLN:O	3:C:204:VAL:HA	2.07	0.54
1:A:476:ILE:CG2	1:A:477:ASP:H	2.19	0.54
2:B:36:HIS:CE1	2:B:40:TYR:CZ	2.96	0.54
5:H:9:GLY:H	5:H:112:THR:HG21	1.72	0.54
5:H:89:GLU:H	5:H:89:GLU:CD	2.11	0.54
6:L:37:GLN:NE2	6:L:39:LYS:HZ1	2.04	0.54
6:L:62:PHE:CD2	6:L:75:ILE:HG12	2.42	0.54
1:A:390:GLY:O	7:A:602:HEA:HMB3	2.07	0.54
2:B:24:SER:HG	2:B:212:TYR:HE2	1.56	0.54
1:A:243:THR:O	1:A:247:MET:HG2	2.08	0.54
1:A:245:LEU:HD23	1:A:256:PHE:CE1	2.42	0.54
2:B:247:LYS:HB2	2:B:247:LYS:HZ3	1.72	0.54
3:C:4:LYS:NZ	4:D:7:THR:CA	2.71	0.54
3:C:140:LEU:HB3	3:C:192:GLU:OE2	2.07	0.54
2:B:125:TYR:N	2:B:125:TYR:CD1	2.76	0.54
3:C:270:ILE:HG22	3:C:271:TRP:N	2.23	0.54
4:D:28:LYS:HD3	4:D:32:TRP:CZ2	2.42	0.54
5:H:10:ASP:CG	5:H:11:LEU:H	2.11	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:67:ARG:HH12	5:H:87:LYS:CE	2.16	0.54
1:A:526:HIS:NE2	2:B:70:ARG:NH1	2.56	0.54
3:C:70:VAL:HG13	3:C:233:ARG:HE	1.72	0.54
3:C:239:MET:HE1	3:C:247:PHE:HB2	1.89	0.54
5:H:52:ASN:HD21	5:H:56:GLY:HA3	1.72	0.54
6:L:89:GLN:HB2	6:L:99:PHE:CD1	2.43	0.54
1:A:62:VAL:HG11	1:A:82:PRO:HA	1.88	0.54
2:B:184:THR:O	2:B:214:GLY:HA3	2.08	0.54
3:C:6:HIS:CE1	3:C:8:TYR:N	2.76	0.54
1:A:367:ILE:HG23	1:A:373:MET:CE	2.38	0.54
2:B:214:GLY:O	2:B:229:ILE:N	2.32	0.54
3:C:160:HIS:NE2	3:C:164:LEU:HD22	2.22	0.54
5:H:48:VAL:O	5:H:61:PRO:HD2	2.07	0.54
1:A:53:MET:HG3	1:A:90:MET:HG2	1.89	0.53
3:C:229:VAL:HG11	12:C:302:PC1:H342	1.89	0.53
6:L:16:GLY:O	6:L:77:SER:HA	2.08	0.53
2:B:160:ASN:HD22	2:B:160:ASN:H	1.54	0.53
3:C:150:LEU:HD22	3:C:181:LEU:HD11	1.90	0.53
1:A:371:THR:CG2	1:A:429:TYR:HD1	2.22	0.53
1:A:527:ALA:HB1	1:A:532:TRP:CD1	2.44	0.53
3:C:243:GLN:NE2	12:C:302:PC1:H132	2.24	0.53
6:L:46:PHE:CZ	6:L:49:TYR:HB3	2.44	0.53
1:A:371:THR:HG21	1:A:429:TYR:CD1	2.43	0.53
1:A:278:GLU:O	1:A:281:ILE:N	2.42	0.53
1:A:418:LEU:HD21	1:A:456:SER:HB3	1.89	0.53
6:L:37:GLN:O	6:L:45:GLN:HG2	2.09	0.53
1:A:333:SER:O	1:A:337:GLN:HG3	2.09	0.53
5:H:8:GLY:O	5:H:18:LEU:HD11	2.09	0.53
5:H:76:LYS:O	5:H:77:ASN:HB2	2.09	0.53
1:A:283:ILE:HD11	1:A:379:PHE:HE1	1.74	0.53
1:A:421:VAL:CG2	7:A:601:HEA:H273	2.39	0.53
1:A:474:ARG:CD	2:B:219:LEU:HD22	2.39	0.53
1:A:412:PHE:HE1	1:A:413:HIS:CE1	2.26	0.52
1:A:101:PHE:CE2	1:A:189:SER:HB2	2.44	0.52
1:A:220:PHE:HB2	1:A:292:HIS:CD2	2.44	0.52
2:B:138:MET:CE	2:B:155:LEU:HD23	2.39	0.52
2:B:113:VAL:O	2:B:128:PRO:HD2	2.08	0.52
3:C:140:LEU:CB	3:C:141:PRO:HD3	2.40	0.52
3:C:234:LEU:HD13	3:C:239:MET:SD	2.49	0.52
1:A:263:ASP:OD1	1:A:265:VAL:HG22	2.10	0.52
3:C:141:PRO:HB3	3:C:269:TYR:CD2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:ARG:NH2	1:A:57:LEU:HD13	2.24	0.52
2:B:97:LEU:HB2	2:B:98:PRO:HD3	1.92	0.52
1:A:51:VAL:O	1:A:55:MET:HG3	2.10	0.52
3:C:177:VAL:HG12	3:C:177:VAL:O	2.10	0.52
1:A:130:LEU:CD1	1:A:195:LEU:HD22	2.39	0.52
3:C:239:MET:CE	3:C:247:PHE:HB2	2.40	0.52
5:H:38:ARG:HD2	5:H:46:GLU:OE2	2.09	0.52
5:H:72:ARG:HH12	5:H:74:ASN:HA	1.75	0.52
2:B:4:LEU:CG	2:B:242:TRP:HD1	2.20	0.52
3:C:30:GLY:CA	3:C:50:MET:HB3	2.40	0.52
3:C:75:THR:O	3:C:75:THR:HG22	2.09	0.52
1:A:216:LYS:HG3	1:A:552:TRP:HZ3	1.75	0.51
2:B:190:VAL:CG1	2:B:202:LEU:HD13	2.28	0.51
3:C:124:ASP:CG	12:C:301:PC1:H152	2.30	0.51
3:C:162:PHE:CE2	3:C:234:LEU:HD11	2.44	0.51
5:H:67:ARG:NH1	5:H:87:LYS:HE3	2.20	0.51
6:L:85:SER:HA	6:L:104:LYS:HA	1.90	0.51
1:A:205:LEU:HB3	4:D:22:THR:HG21	1.93	0.51
2:B:172:VAL:O	2:B:202:LEU:HG	2.09	0.51
5:H:12:VAL:O	5:H:116:VAL:HA	2.09	0.51
1:A:374:LEU:HD13	1:A:449:PHE:CD1	2.45	0.51
2:B:140:GLU:HA	2:B:154:TYR:HE1	1.75	0.51
3:C:244:HIS:ND1	3:C:244:HIS:N	2.58	0.51
1:A:127:PHE:N	1:A:127:PHE:CD2	2.76	0.51
4:D:20:GLN:OE1	4:D:20:GLN:HA	2.11	0.51
5:H:49:ALA:HB1	5:H:70:ILE:HB	1.93	0.51
1:A:103:VAL:HG21	7:A:601:HEA:HBC2	1.91	0.51
1:A:324:ALA:HB3	1:A:340:PHE:CD2	2.44	0.51
1:A:438:ARG:HB3	1:A:514:GLY:HA3	1.92	0.51
1:A:456:SER:HA	1:A:459:ILE:CD1	2.41	0.51
6:L:36:TYR:O	6:L:86:TYR:HA	2.09	0.51
1:A:63:GLN:O	1:A:80:CYS:SG	2.69	0.51
1:A:301:PRO:O	1:A:361:THR:HG23	2.11	0.51
1:A:406:TYR:HE2	1:A:472:PRO:O	1.94	0.51
7:A:602:HEA:H273	7:A:602:HEA:C26	2.40	0.51
6:L:61:ARG:O	6:L:75:ILE:HA	2.11	0.51
1:A:334:LEU:HD21	2:B:101:PHE:CD1	2.45	0.51
3:C:170:THR:O	3:C:174:GLY:N	2.35	0.51
3:C:158:ALA:O	3:C:171:THR:HG23	2.10	0.51
1:A:174:GLU:HB3	1:A:249:ARG:HH22	1.75	0.51
1:A:437:GLY:HA3	1:A:537:PRO:HD3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:119:HIS:CD2	2:B:124:SER:HB3	2.46	0.51
5:H:29:PHE:O	5:H:72:ARG:NH2	2.44	0.51
1:A:37:PHE:O	1:A:41:ILE:HG12	2.11	0.50
3:C:213:THR:HA	3:C:264:LEU:HD13	1.92	0.50
1:A:375:TRP:HZ2	1:A:448:HIS:ND1	2.09	0.50
2:B:110:PRO:HG3	2:B:171:LEU:HD22	1.93	0.50
3:C:81:VAL:HG23	3:C:82:VAL:H	1.76	0.50
1:A:542:THR:HG22	1:A:543:PHE:CD2	2.47	0.50
3:C:140:LEU:HB2	3:C:141:PRO:HD3	1.92	0.50
3:C:158:ALA:HB2	3:C:174:GLY:HA3	1.93	0.50
1:A:96:VAL:O	1:A:100:PHE:HB2	2.11	0.50
1:A:306:LEU:HB3	1:A:307:PRO:HD3	1.94	0.50
1:A:337:GLN:O	1:A:341:MET:HB2	2.11	0.50
3:C:90:PHE:CE2	3:C:253:TYR:HB2	2.46	0.50
3:C:226:PHE:HA	12:C:302:PC1:H361	1.92	0.50
3:C:226:PHE:CE2	3:C:250:ALA:HA	2.46	0.50
3:C:265:PHE:O	3:C:269:TYR:HB2	2.12	0.50
5:H:47:TRP:NE1	5:H:50:SER:OG	2.45	0.50
6:L:107:ILE:HD12	6:L:107:ILE:N	2.24	0.50
3:C:234:LEU:C	3:C:236:LYS:H	2.15	0.50
1:A:181:LEU:CD1	3:C:32:VAL:HG11	2.42	0.50
1:A:388:VAL:CG1	2:B:42:ILE:HB	2.42	0.50
3:C:216:HIS:HD2	3:C:260:VAL:CG1	2.22	0.50
1:A:104:ILE:HG23	1:A:108:PHE:CB	2.42	0.50
1:A:336:GLN:OE1	12:C:301:PC1:H12	2.12	0.50
1:A:374:LEU:HB3	1:A:449:PHE:CD1	2.47	0.50
1:A:418:LEU:CD2	1:A:456:SER:HB3	2.41	0.50
6:L:12:SER:HB3	6:L:108:LYS:HB2	1.94	0.50
5:H:9:GLY:HA3	5:H:112:THR:HG22	1.94	0.50
5:H:10:ASP:CG	5:H:11:LEU:N	2.65	0.50
5:H:68:PHE:HA	5:H:82:GLN:O	2.12	0.50
1:A:98:MET:SD	7:A:601:HEA:HMC3	2.51	0.50
7:A:601:HEA:HMC1	7:A:601:HEA:HBC1	1.92	0.50
1:A:68:GLU:OE2	1:A:79:GLU:HB3	2.12	0.49
3:C:16:TRP:HE3	3:C:61:VAL:HG13	1.78	0.49
3:C:163:VAL:HB	3:C:164:LEU:HD12	1.93	0.49
1:A:400:ARG:HH11	1:A:400:ARG:CG	2.25	0.49
1:A:406:TYR:HB3	1:A:463:GLN:HB3	1.94	0.49
1:A:502:PHE:O	1:A:506:ILE:HG13	2.12	0.49
2:B:4:LEU:CD1	2:B:242:TRP:NE1	2.64	0.49
1:A:111:PHE:O	1:A:220:PHE:CZ	2.63	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:132:ILE:HD11	3:C:202:ASP:HB3	1.95	0.49
6:L:37:GLN:NE2	6:L:39:LYS:NZ	2.59	0.49
1:A:48:CYS:O	1:A:51:VAL:HG22	2.13	0.49
1:A:65:MET:O	1:A:83:ASN:ND2	2.45	0.49
1:A:247:MET:C	1:A:249:ARG:H	2.15	0.49
3:C:230:CYS:O	3:C:234:LEU:HB2	2.12	0.49
3:C:234:LEU:CD1	3:C:239:MET:SD	3.01	0.49
3:C:253:TYR:O	3:C:256:PHE:HB3	2.13	0.49
1:A:478:TYR:CD1	1:A:482:PHE:HB2	2.47	0.49
1:A:377:PHE:HE1	2:B:53:LEU:HD13	1.78	0.49
2:B:39:LEU:HA	2:B:42:ILE:HG12	1.94	0.49
3:C:168:ARG:NH2	3:C:234:LEU:HD12	2.28	0.49
6:L:32:TYR:CD2	6:L:92:TYR:HB2	2.48	0.49
3:C:4:LYS:HE2	4:D:8:ASP:N	2.27	0.49
3:C:33:ALA:HA	3:C:38:ILE:HG13	1.95	0.49
1:A:474:ARG:HD2	2:B:219:LEU:HD22	1.95	0.48
2:B:36:HIS:CE1	2:B:40:TYR:OH	2.66	0.48
1:A:280:TYR:CE1	1:A:315:ILE:HG23	2.48	0.48
1:A:392:VAL:CG2	2:B:42:ILE:HD13	2.43	0.48
1:A:126:ALA:C	1:A:127:PHE:HD2	2.17	0.48
5:H:24:ALA:HB1	5:H:27:PHE:CE1	2.48	0.48
1:A:54:ARG:HH21	1:A:57:LEU:HB3	1.78	0.48
1:A:58:GLN:HG3	1:A:487:ASN:HB2	1.95	0.48
1:A:438:ARG:HG2	1:A:511:LEU:O	2.12	0.48
1:A:473:ARG:HG3	1:A:474:ARG:HG3	1.94	0.48
3:C:119:ASP:O	3:C:122:ILE:HG12	2.13	0.48
1:A:267:TYR:HE2	1:A:271:LEU:HD22	1.75	0.48
3:C:176:ILE:C	3:C:178:ALA:H	2.15	0.48
1:A:65:MET:HB3	1:A:83:ASN:ND2	2.27	0.48
1:A:445:GLY:O	1:A:448:HIS:N	2.47	0.48
1:A:47:VAL:HG11	7:A:601:HEA:H263	1.96	0.48
1:A:104:ILE:HG23	1:A:108:PHE:HB3	1.96	0.48
3:C:34:TRP:HE1	3:C:48:PRO:HG3	1.77	0.48
6:L:87:TYR:CD2	6:L:102:GLY:HA3	2.48	0.48
1:A:339:TYR:CE2	12:C:301:PC1:H3A1	2.49	0.48
1:A:432:ILE:HG21	1:A:440:TYR:HB3	1.96	0.48
1:A:540:GLU:HG2	1:A:541:HIS:HD2	1.79	0.48
1:A:274:PHE:C	1:A:277:PRO:HD2	2.33	0.48
1:A:412:PHE:CD2	7:A:602:HEA:HAD1	2.48	0.48
1:A:469:GLN:NE2	2:B:14:VAL:H	2.10	0.48
2:B:180:ILE:CG2	2:B:218:GLU:HG2	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:218:GLU:H	2:B:224:HIS:HE1	1.62	0.48
5:H:64:VAL:HG13	5:H:68:PHE:HB2	1.94	0.48
6:L:85:SER:HB3	6:L:104:LYS:HG3	1.96	0.48
1:A:133:LEU:O	1:A:137:MET:CG	2.62	0.48
1:A:393:LEU:HD21	1:A:407:TYR:HD2	1.79	0.48
1:A:519:VAL:HG13	1:A:520:PRO:HD2	1.96	0.48
3:C:69:VAL:CG1	12:C:302:PC1:H32	2.44	0.48
3:C:191:TYR:CE2	3:C:195:HIS:NE2	2.82	0.48
1:A:380:LEU:HD23	2:B:53:LEU:CD2	2.44	0.47
1:A:385:VAL:O	1:A:389:THR:HG23	2.14	0.47
1:A:469:GLN:HE21	2:B:14:VAL:H	1.61	0.47
3:C:11:LEU:HD12	3:C:12:PRO:HD2	1.96	0.47
5:H:51:ILE:HD11	5:H:55:GLY:HA2	1.95	0.47
1:A:115:PHE:O	1:A:119:HIS:ND1	2.47	0.47
1:A:206:ASN:HD22	1:A:207:MET:HG3	1.78	0.47
2:B:38:VAL:HG23	2:B:39:LEU:N	2.29	0.47
6:L:71:PHE:N	6:L:71:PHE:CD1	2.82	0.47
1:A:456:SER:HA	1:A:459:ILE:HD12	1.94	0.47
2:B:198:ARG:HE	3:C:116:MET:CE	2.27	0.47
3:C:4:LYS:NZ	4:D:7:THR:CB	2.77	0.47
5:H:86:LEU:HB3	5:H:116:VAL:HG21	1.96	0.47
1:A:57:LEU:HD11	1:A:87:TRP:HH2	1.78	0.47
3:C:81:VAL:HG23	3:C:82:VAL:HG23	1.97	0.47
3:C:119:ASP:CB	3:C:123:LYS:HB2	2.44	0.47
1:A:355:VAL:HA	1:A:358:TRP:CE3	2.48	0.47
3:C:205:TYR:O	3:C:209:PHE:N	2.47	0.47
1:A:230:LEU:HD21	1:A:316:GLY:HA2	1.96	0.47
1:A:322:VAL:HG12	1:A:343:ALA:CB	2.45	0.47
1:A:409:VAL:HG11	7:A:601:HEA:HAA2	1.97	0.47
2:B:67:VAL:O	2:B:67:VAL:HG23	2.14	0.47
2:B:74:ASN:HD22	2:B:76:PRO:HD2	1.79	0.47
2:B:98:PRO:O	2:B:102:ARG:HG3	2.14	0.47
2:B:173:GLN:HG3	2:B:173:GLN:O	2.15	0.47
3:C:198:PHE:HZ	3:C:209:PHE:CD2	2.33	0.47
3:C:270:ILE:HD13	3:C:270:ILE:HA	1.75	0.47
4:D:31:THR:O	4:D:35:ILE:HG12	2.14	0.47
1:A:129:ARG:HB3	3:C:11:LEU:CD2	2.45	0.47
1:A:140:CYS:O	1:A:144:LEU:HB2	2.14	0.47
1:A:171:SER:O	1:A:249:ARG:NH1	2.48	0.47
2:B:167:GLY:HA2	5:H:102:TYR:CZ	2.50	0.47
5:H:97:VAL:CG2	5:H:105:MET:HG2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:ARG:NH1	1:A:22:TRP:CZ2	2.83	0.47
1:A:34:LEU:HD23	1:A:135:TYR:CD2	2.49	0.47
1:A:67:LEU:HD23	1:A:67:LEU:C	2.34	0.47
1:A:204:PHE:CE1	1:A:217:VAL:HG11	2.50	0.47
3:C:25:PHE:O	3:C:29:THR:HG23	2.15	0.47
3:C:127:TRP:CZ2	3:C:205:TYR:HD2	2.32	0.47
3:C:129:PRO:HG2	3:C:203:THR:CG2	2.34	0.47
1:A:39:ALA:HB1	1:A:102:VAL:O	2.14	0.46
1:A:404:ASP:HA	1:A:473:ARG:HD2	1.97	0.46
1:A:98:MET:SD	7:A:601:HEA:C1C	3.03	0.46
1:A:121:GLY:HA2	1:A:543:PHE:CE2	2.50	0.46
12:C:302:PC1:H132	12:C:302:PC1:H112	1.69	0.46
1:A:238:LEU:HB2	1:A:274:PHE:CG	2.50	0.46
1:A:439:GLN:O	1:A:510:THR:HG23	2.15	0.46
1:A:57:LEU:O	1:A:486:ASN:HB3	2.16	0.46
1:A:106:ALA:CB	7:A:601:HEA:H253	2.44	0.46
1:A:282:ILE:HG22	1:A:283:ILE:N	2.30	0.46
2:B:198:ARG:HE	3:C:116:MET:HE2	1.80	0.46
2:B:227:MET:O	2:B:227:MET:HG3	2.16	0.46
3:C:191:TYR:HA	3:C:194:SER:OG	2.16	0.46
3:C:69:VAL:HA	3:C:72:GLU:OE2	2.16	0.46
3:C:243:GLN:CD	12:C:302:PC1:H132	2.35	0.46
1:A:36:LEU:HD22	1:A:110:GLY:HA3	1.97	0.46
1:A:164:TRP:CD2	1:A:165:VAL:HG13	2.51	0.46
1:A:299:LYS:O	2:B:70:ARG:NH2	2.49	0.46
3:C:217:GLY:O	3:C:220:VAL:HG12	2.15	0.46
1:A:464:HIS:O	1:A:468:ARG:HG3	2.15	0.46
1:A:469:GLN:NE2	2:B:13:PRO:HA	2.31	0.46
1:A:324:ALA:C	1:A:326:HIS:H	2.18	0.46
1:A:353:ILE:O	1:A:357:SER:HB2	2.15	0.46
1:A:469:GLN:OE1	2:B:19:ASN:O	2.34	0.46
3:C:220:VAL:O	3:C:224:THR:HG23	2.16	0.46
5:H:39:GLN:HG2	5:H:43:LYS:HA	1.97	0.46
5:H:89:GLU:CD	5:H:89:GLU:N	2.69	0.46
6:L:89:GLN:HB2	6:L:99:PHE:CE1	2.51	0.46
1:A:123:PRO:O	1:A:542:THR:HB	2.16	0.46
1:A:241:ALA:HB2	1:A:270:ILE:CG2	2.45	0.46
7:A:602:HEA:CB	7:A:602:HEA:HMC1	2.46	0.46
7:A:602:HEA:H212	7:A:602:HEA:H271	1.61	0.46
3:C:151:SER:O	3:C:155:VAL:HG23	2.15	0.46
12:C:301:PC1:C22	12:C:301:PC1:H32	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:32:TRP:N	4:D:32:TRP:CD1	2.80	0.46
1:A:69:GLY:O	1:A:71:ARG:NH1	2.49	0.45
1:A:136:TRP:HA	1:A:136:TRP:CE3	2.50	0.45
1:A:279:VAL:HB	7:A:602:HEA:CAC	2.41	0.45
1:A:356:PHE:CD1	2:B:81:TRP:HB2	2.46	0.45
1:A:396:ALA:N	1:A:397:PRO:HD2	2.31	0.45
3:C:33:ALA:HB2	3:C:38:ILE:HD12	1.97	0.45
1:A:174:GLU:HB3	1:A:249:ARG:NH2	2.30	0.45
1:A:177:TYR:CE1	3:C:38:ILE:HA	2.52	0.45
1:A:204:PHE:HE1	1:A:221:ALA:HB1	1.81	0.45
1:A:227:THR:HG22	1:A:231:ILE:HD11	1.97	0.45
1:A:429:TYR:HH	1:A:503:PHE:HD1	1.56	0.45
5:H:4:LEU:HD23	5:H:24:ALA:HB2	1.96	0.45
1:A:262:GLY:O	1:A:264:PRO:HD3	2.16	0.45
1:A:179:MET:HB2	1:A:249:ARG:NH2	2.31	0.45
1:A:280:TYR:CD1	1:A:315:ILE:CG2	3.00	0.45
1:A:47:VAL:HG23	1:A:98:MET:HE1	1.98	0.45
7:A:601:HEA:HMC1	7:A:601:HEA:CBC	2.47	0.45
2:B:140:GLU:HA	2:B:154:TYR:CE1	2.51	0.45
3:C:225:ILE:HG22	12:C:302:PC1:H382	1.97	0.45
6:L:47:LEU:HA	6:L:58:VAL:HG21	1.98	0.45
1:A:18:PHE:C	1:A:20:THR:H	2.20	0.45
3:C:180:ILE:HD12	3:C:180:ILE:HA	1.88	0.45
5:H:5:GLN:HB3	5:H:23:ALA:HB3	1.99	0.45
6:L:98:THR:HG22	6:L:99:PHE:N	2.32	0.45
1:A:104:ILE:HD13	1:A:104:ILE:HA	1.71	0.45
2:B:127:TYR:CD1	2:B:132:VAL:HB	2.52	0.45
2:B:61:ASN:O	2:B:65:ASN:N	2.49	0.45
2:B:183:TRP:CD1	2:B:229:ILE:HD13	2.52	0.45
3:C:2:HIS:C	3:C:3:VAL:HG13	2.36	0.45
1:A:141:GLY:O	1:A:145:GLY:N	2.49	0.45
1:A:322:VAL:HG12	1:A:343:ALA:HB1	1.99	0.45
1:A:325:HIS:O	7:A:602:HEA:HAA1	2.17	0.45
3:C:124:ASP:OD1	12:C:301:PC1:H152	2.17	0.45
6:L:88:CYS:O	6:L:100:GLY:N	2.48	0.45
1:A:22:TRP:HE3	1:A:34:LEU:HD13	1.82	0.44
1:A:371:THR:HB	1:A:372:PRO:HD3	1.99	0.44
1:A:546:LEU:HA	1:A:547:PRO:HD3	1.77	0.44
1:A:101:PHE:O	1:A:102:VAL:HG23	2.16	0.44
1:A:441:PRO:HA	1:A:515:LYS:HZ1	1.82	0.44
2:B:163:VAL:HG21	2:B:242:TRP:CD2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:190:VAL:HG12	2:B:202:LEU:HD22	1.99	0.44
6:L:11:LEU:HD21	6:L:19:VAL:HG21	1.98	0.44
1:A:54:ARG:HD3	1:A:490:SER:OG	2.18	0.44
1:A:254:GLN:HG3	3:C:202:ASP:C	2.38	0.44
2:B:71:PHE:N	2:B:71:PHE:CD1	2.85	0.44
3:C:129:PRO:CB	3:C:203:THR:HG21	2.47	0.44
6:L:24:ARG:HA	6:L:69:THR:O	2.17	0.44
1:A:39:ALA:HB3	7:A:601:HEA:H252	1.99	0.44
1:A:260:GLY:O	3:C:203:THR:HG22	2.17	0.44
2:B:63:ARG:C	2:B:65:ASN:H	2.20	0.44
2:B:166:VAL:HG22	2:B:167:GLY:N	2.32	0.44
1:A:459:ILE:HD11	1:A:496:SER:OG	2.17	0.44
3:C:156:THR:O	3:C:156:THR:HG22	2.18	0.44
5:H:41:PRO:HB2	5:H:42:GLU:OE1	2.17	0.44
5:H:81:LEU:HD13	5:H:83:MET:CG	2.47	0.44
1:A:379:PHE:HB2	1:A:422:PHE:HB3	1.99	0.44
2:B:63:ARG:HA	2:B:63:ARG:NE	2.32	0.44
1:A:19:PHE:CG	1:A:19:PHE:O	2.71	0.44
1:A:150:LEU:HA	1:A:150:LEU:HD13	1.74	0.44
3:C:28:LEU:C	3:C:30:GLY:N	2.72	0.44
5:H:33:THR:HG21	5:H:103:TYR:HE1	1.83	0.44
5:H:72:ARG:NH1	5:H:74:ASN:CG	2.71	0.44
1:A:127:PHE:N	1:A:127:PHE:HD2	2.15	0.44
1:A:459:ILE:O	1:A:489:SER:OG	2.34	0.44
1:A:98:MET:O	1:A:103:VAL:CG2	2.65	0.43
1:A:208:ARG:NE	1:A:213:THR:O	2.51	0.43
2:B:63:ARG:HH22	2:B:66:PRO:HB3	1.83	0.43
3:C:90:PHE:HE1	12:C:302:PC1:H271	1.83	0.43
5:H:5:GLN:O	5:H:22:CYS:CA	2.63	0.43
5:H:59:TYR:HB2	6:L:95:PRO:HB2	2.00	0.43
1:A:390:GLY:C	7:A:602:HEA:HMB3	2.39	0.43
1:A:406:TYR:CE2	1:A:472:PRO:O	2.71	0.43
1:A:460:PHE:HD2	1:A:463:GLN:OE1	2.01	0.43
3:C:82:VAL:O	3:C:86:LEU:HD12	2.18	0.43
6:L:83:PHE:HE2	6:L:106:GLU:O	2.01	0.43
1:A:227:THR:O	1:A:231:ILE:HG13	2.19	0.43
1:A:374:LEU:HD13	1:A:449:PHE:HD1	1.83	0.43
2:B:163:VAL:HG12	2:B:232:LYS:HB2	2.00	0.43
1:A:308:MET:SD	1:A:354:LYS:HA	2.59	0.43
1:A:462:PRO:O	1:A:465:PHE:HB2	2.18	0.43
2:B:79:VAL:HA	2:B:82:THR:HG22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:145:ALA:C	2:B:147:ALA:H	2.22	0.43
1:A:297:PHE:CE2	1:A:370:LYS:HB2	2.52	0.43
1:A:325:HIS:HB2	7:A:602:HEA:CMA	2.49	0.43
1:A:369:PHE:CZ	2:B:57:ILE:HG12	2.53	0.43
1:A:455:GLY:O	1:A:459:ILE:HG13	2.18	0.43
2:B:206:VAL:HG11	2:B:233:ALA:HB2	1.99	0.43
6:L:86:TYR:O	6:L:102:GLY:HA2	2.18	0.43
1:A:21:ARG:NH1	1:A:22:TRP:HZ2	2.17	0.43
1:A:276:HIS:NE2	1:A:280:TYR:CD2	2.86	0.43
1:A:393:LEU:HD21	1:A:407:TYR:CD2	2.54	0.43
3:C:144:ASN:HB3	3:C:185:PHE:HE1	1.83	0.43
12:C:301:PC1:H32	12:C:301:PC1:H321	1.77	0.43
1:A:238:LEU:HD22	1:A:274:PHE:CD1	2.54	0.43
1:A:410:ALA:HB3	1:A:464:HIS:CD2	2.53	0.43
1:A:519:VAL:CG1	1:A:520:PRO:HD2	2.48	0.43
3:C:209:PHE:HE1	3:C:269:TYR:CE1	2.23	0.43
1:A:47:VAL:HG12	1:A:47:VAL:O	2.18	0.43
1:A:106:ALA:HB1	7:A:601:HEA:H253	2.00	0.43
1:A:219:LEU:HD23	1:A:219:LEU:HA	1.76	0.43
5:H:41:PRO:HD3	5:H:91:THR:O	2.18	0.43
1:A:84:GLY:CA	2:B:222:ILE:HG13	2.49	0.43
1:A:241:ALA:HA	1:A:244:MET:HE3	2.01	0.43
1:A:538:PRO:HA	1:A:539:PRO:HD3	1.81	0.43
2:B:80:ILE:HD13	2:B:80:ILE:HA	1.89	0.43
2:B:144:LEU:HD21	2:B:154:TYR:HA	2.01	0.43
3:C:90:PHE:CZ	3:C:253:TYR:HB2	2.53	0.43
1:A:26:THR:HG23	1:A:128:PRO:HB2	2.01	0.42
1:A:84:GLY:N	2:B:222:ILE:HG13	2.34	0.42
1:A:85:HIS:HE1	1:A:154:GLY:HA3	1.83	0.42
1:A:85:HIS:ND1	1:A:155:ASN:ND2	2.66	0.42
1:A:414:TYR:HA	1:A:418:LEU:HB2	2.01	0.42
2:B:27:LEU:HD12	2:B:27:LEU:H	1.83	0.42
3:C:28:LEU:O	3:C:31:ALA:N	2.52	0.42
3:C:122:ILE:HG13	3:C:123:LYS:HG3	2.01	0.42
1:A:18:PHE:O	1:A:20:THR:N	2.48	0.42
1:A:162:VAL:HG13	1:A:174:GLU:OE1	2.19	0.42
2:B:198:ARG:NH2	12:C:301:PC1:O12	2.52	0.42
3:C:39:THR:HG22	3:C:44:PRO:HB3	2.01	0.42
3:C:233:ARG:O	3:C:238:GLN:HG3	2.19	0.42
6:L:61:ARG:HB3	6:L:76:ASN:O	2.19	0.42
1:A:219:LEU:HD11	1:A:302:ILE:HG21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:509:TYR:CD2	1:A:509:TYR:C	2.91	0.42
5:H:87:LYS:HG3	5:H:89:GLU:HG2	2.02	0.42
1:A:21:ARG:HD3	1:A:22:TRP:CE2	2.55	0.42
5:H:64:VAL:HG22	5:H:68:PHE:CE1	2.55	0.42
6:L:51:ALA:O	6:L:64:GLY:HA3	2.19	0.42
3:C:86:LEU:HD13	12:C:302:PC1:O22	2.19	0.42
5:H:5:GLN:HA	5:H:110:GLN:OE1	2.19	0.42
1:A:22:TRP:CE3	1:A:34:LEU:HD13	2.54	0.42
1:A:339:TYR:CD2	12:C:301:PC1:H381	2.55	0.42
1:A:437:GLY:O	1:A:517:VAL:HG23	2.19	0.42
3:C:226:PHE:CD2	3:C:250:ALA:HA	2.54	0.42
5:H:51:ILE:HB	5:H:70:ILE:HG21	2.02	0.42
5:H:59:TYR:N	5:H:59:TYR:CD2	2.87	0.42
2:B:138:MET:HE1	2:B:155:LEU:HD23	2.01	0.42
5:H:17:SER:O	5:H:18:LEU:HB2	2.19	0.42
1:A:417:SER:O	1:A:418:LEU:HD23	2.20	0.42
2:B:36:HIS:HE1	2:B:40:TYR:OH	2.02	0.42
2:B:222:ILE:HG23	2:B:223:ASN:N	2.35	0.42
3:C:32:VAL:HB	3:C:38:ILE:HD11	2.01	0.42
3:C:144:ASN:HB3	3:C:185:PHE:CE1	2.55	0.42
5:H:47:TRP:CZ2	5:H:50:SER:OG	2.72	0.42
1:A:219:LEU:HD21	1:A:305:TYR:CE1	2.55	0.42
2:B:9:VAL:HG22	2:B:211:VAL:HB	2.02	0.42
2:B:238:LYS:O	2:B:241:ALA:HB3	2.19	0.42
12:C:301:PC1:H3I3	12:C:301:PC1:H2H1	2.02	0.42
5:H:101:TYR:O	5:H:102:TYR:HB2	2.20	0.42
6:L:79:LEU:HD22	6:L:80:PRO:HD3	2.01	0.42
1:A:238:LEU:HD22	1:A:274:PHE:CE2	2.54	0.41
1:A:248:ASP:HB3	1:A:255:PHE:HB2	2.02	0.41
1:A:381:PHE:CE1	2:B:50:CYS:SG	3.13	0.41
3:C:79:THR:OG1	3:C:82:VAL:HG23	2.20	0.41
6:L:36:TYR:N	6:L:87:TYR:O	2.53	0.41
1:A:93:TYR:O	1:A:97:LEU:HG	2.19	0.41
2:B:158:THR:HB	2:B:159:ASP:H	1.58	0.41
1:A:28:HIS:HD2	1:A:113:ASN:O	2.02	0.41
1:A:280:TYR:O	1:A:284:LEU:HB2	2.20	0.41
2:B:61:ASN:OD1	2:B:64:ALA:HB3	2.19	0.41
3:C:78:HIS:HA	3:C:82:VAL:HG11	2.03	0.41
6:L:12:SER:HA	6:L:106:GLU:O	2.20	0.41
1:A:234:SER:HB2	1:A:274:PHE:HA	2.01	0.41
1:A:404:ASP:HA	1:A:473:ARG:CD	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:537:PRO:HA	1:A:538:PRO:HD3	1.87	0.41
2:B:62:ARG:CZ	2:B:63:ARG:HG2	2.50	0.41
3:C:11:LEU:CD1	3:C:12:PRO:HD2	2.51	0.41
3:C:270:ILE:O	3:C:271:TRP:C	2.59	0.41
1:A:104:ILE:O	1:A:105:PRO:C	2.55	0.41
1:A:278:GLU:O	1:A:280:TYR:N	2.53	0.41
1:A:434:LYS:HE2	1:A:532:TRP:CZ3	2.56	0.41
3:C:127:TRP:HA	3:C:127:TRP:CE3	2.55	0.41
1:A:54:ARG:NH1	7:A:601:HEA:OMA	2.54	0.41
1:A:366:SER:HA	2:B:65:ASN:O	2.21	0.41
1:A:425:PHE:O	1:A:427:GLY:N	2.54	0.41
1:A:438:ARG:HD2	1:A:438:ARG:N	2.35	0.41
1:A:526:HIS:CE1	2:B:70:ARG:HH12	2.38	0.41
2:B:91:ALA:O	2:B:94:ALA:HB3	2.20	0.41
2:B:162:VAL:HG13	2:B:231:VAL:HA	2.02	0.41
1:A:35:TYR:CE2	1:A:138:TYR:CD2	3.09	0.41
3:C:238:GLN:O	12:C:302:PC1:H153	2.20	0.41
6:L:39:LYS:HA	6:L:39:LYS:HE3	2.01	0.41
6:L:47:LEU:O	6:L:54:LEU:HA	2.21	0.41
1:A:177:TYR:OH	3:C:38:ILE:HG23	2.20	0.41
1:A:234:SER:O	1:A:237:VAL:HG23	2.20	0.41
1:A:257:ASP:HA	1:A:258:PRO:HD3	1.75	0.41
1:A:441:PRO:HG2	1:A:444:ALA:HB3	2.03	0.41
3:C:113:LEU:HD13	3:C:114:TYR:CE1	2.56	0.41
3:C:143:ILE:O	3:C:147:ILE:HG13	2.21	0.41
3:C:158:ALA:CB	3:C:175:LEU:HD22	2.49	0.41
6:L:11:LEU:HD21	6:L:19:VAL:CG2	2.51	0.41
1:A:126:ALA:N	1:A:207:MET:SD	2.94	0.41
2:B:10:ILE:HB	2:B:212:TYR:CE2	2.55	0.41
2:B:43:THR:O	2:B:47:ILE:HG12	2.21	0.41
2:B:75:THR:OG1	2:B:76:PRO:HD3	2.20	0.41
2:B:113:VAL:O	2:B:113:VAL:HG12	2.21	0.41
2:B:159:ASP:C	2:B:161:PRO:HD3	2.28	0.41
2:B:215:GLN:HE21	2:B:215:GLN:HB3	1.69	0.41
3:C:122:ILE:HG13	3:C:123:LYS:N	2.36	0.41
1:A:322:VAL:HB	1:A:344:THR:OG1	2.21	0.41
1:A:501:LEU:HD23	1:A:501:LEU:HA	1.87	0.41
2:B:159:ASP:HB2	2:B:160:ASN:HD22	1.86	0.41
3:C:15:ILE:HD12	3:C:19:PHE:CZ	2.56	0.41
3:C:81:VAL:CG2	3:C:82:VAL:N	2.84	0.41
1:A:349:VAL:HB	1:A:350:PRO:CD	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:VAL:C	1:A:410:ALA:H	2.23	0.40
2:B:182:ALA:HB3	2:B:217:SER:H	1.87	0.40
3:C:86:LEU:HD22	12:C:302:PC1:O22	2.22	0.40
3:C:110:LYS:HD3	3:C:110:LYS:C	2.42	0.40
2:B:24:SER:OG	2:B:212:TYR:CE2	2.74	0.40
2:B:30:ASP:HB3	2:B:99:ILE:HG23	2.03	0.40
6:L:6:GLN:HE21	6:L:6:GLN:HB3	1.78	0.40
6:L:22:THR:HA	6:L:72:SER:HA	2.02	0.40
1:A:179:MET:HG3	1:A:249:ARG:NH1	2.32	0.40
3:C:144:ASN:HD21	3:C:188:LEU:HB3	1.87	0.40
1:A:136:TRP:HB3	3:C:21:ALA:HB2	2.03	0.40
3:C:75:THR:O	3:C:75:THR:CG2	2.70	0.40
3:C:172:ILE:HD13	3:C:235:LEU:HD12	2.04	0.40
6:L:21:ILE:CG1	6:L:73:LEU:HB3	2.47	0.40
1:A:136:TRP:HB3	3:C:21:ALA:CB	2.52	0.40
1:A:217:VAL:CG1	1:A:221:ALA:HB3	2.51	0.40
1:A:378:GLY:HA3	1:A:422:PHE:HE2	1.87	0.40
1:A:379:PHE:CD1	1:A:419:GLY:O	2.69	0.40
1:A:395:GLN:OE1	2:B:92:ILE:CG2	2.69	0.40
1:A:434:LYS:N	1:A:522:TYR:OH	2.55	0.40
3:C:98:VAL:O	3:C:102:VAL:HG23	2.22	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	536/538 (100%)	447 (83%)	71 (13%)	18 (3%)	3	17
2	B	250/252 (99%)	198 (79%)	47 (19%)	5 (2%)	6	29
3	C	271/273 (99%)	215 (79%)	51 (19%)	5 (2%)	7	32
4	D	41/43 (95%)	33 (80%)	5 (12%)	3 (7%)	1	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	H	117/119 (98%)	99 (85%)	16 (14%)	2 (2%)	7	33
6	L	106/108 (98%)	92 (87%)	13 (12%)	1 (1%)	14	49
All	All	1321/1333 (99%)	1084 (82%)	203 (15%)	34 (3%)	4	23

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	18	PHE
1	A	213	THR
1	A	442	GLU
1	A	19	PHE
1	A	102	VAL
1	A	162	VAL
1	A	369	PHE
1	A	480	VAL
2	B	160	ASN
3	C	3	VAL
4	D	47	ALA
1	A	112	GLY
1	A	304	GLY
1	A	322	VAL
1	A	513	ALA
2	B	62	ARG
2	B	152	ASP
5	H	102	TYR
6	L	51	ALA
1	A	126	ALA
1	A	278	GLU
1	A	512	PHE
2	B	120	GLN
3	C	46	GLU
4	D	11	HIS
1	A	26	THR
2	B	66	PRO
3	C	34	TRP
4	D	48	ASN
5	H	54	GLY
3	C	177	VAL
1	A	279	VAL
3	C	270	ILE
1	A	409	VAL

### 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	441/441 (100%)	387 (88%)	54 (12%)	4	18
2	B	211/211 (100%)	183 (87%)	28 (13%)	3	15
3	C	220/220 (100%)	197 (90%)	23 (10%)	5	23
4	D	34/34 (100%)	28 (82%)	6 (18%)	1	8
5	H	101/101 (100%)	91 (90%)	10 (10%)	6	26
6	L	92/92 (100%)	80 (87%)	12 (13%)	3	16
All	All	1099/1099 (100%)	966 (88%)	133 (12%)	4	18

All (133) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	PHE
1	A	36	LEU
1	A	48	CYS
1	A	54	ARG
1	A	62	VAL
1	A	68	GLU
1	A	72	LEU
1	A	73	ILE
1	A	83	ASN
1	A	90	MET
1	A	94	HIS
1	A	98	MET
1	A	104	ILE
1	A	105	PRO
1	A	119	HIS
1	A	124	ASP
1	A	127	PHE
1	A	131	ASN
1	A	132	ASN
1	A	138	TYR
1	A	139	VAL
1	A	149	LEU

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Mol	Chain	Res	Type
1	A	155	ASN
1	A	158	MET
1	A	162	VAL
1	A	164	TRP
1	A	166	LEU
1	A	177	TYR
1	A	187	HIS
1	A	216	LYS
1	A	235	LEU
1	A	255	PHE
1	A	274	PHE
1	A	279	VAL
1	A	308	MET
1	A	345	MET
1	A	370	LYS
1	A	377	PHE
1	A	388	VAL
1	A	393	LEU
1	A	400	ARG
1	A	404	ASP
1	A	412	PHE
1	A	422	PHE
1	A	446	GLN
1	A	458	LEU
1	A	480	VAL
1	A	487	ASN
1	A	491	ILE
1	A	495	ILE
1	A	508	PHE
1	A	516	ARG
1	A	522	TYR
1	A	548	LYS
2	B	3	VAL
2	B	14	VAL
2	B	29	HIS
2	B	49	VAL
2	B	54	LEU
2	B	63	ARG
2	B	65	ASN
2	B	70	ARG
2	B	71	PHE
2	B	74	ASN

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Mol	Chain	Res	Type
2	B	79	VAL
2	B	81	TRP
2	B	103	SER
2	B	111	ASP
2	B	130	ASP
2	B	142	GLU
2	B	152	ASP
2	B	156	LEU
2	B	159	ASP
2	B	160	ASN
2	B	161	PRO
2	B	174	VAL
2	B	178	ASP
2	B	198	ARG
2	B	215	GLN
2	B	217	SER
2	B	243	LEU
2	B	247	LYS
3	C	2	HIS
3	C	4	LYS
3	C	5	ASN
3	C	6	HIS
3	C	15	ILE
3	C	26	VAL
3	C	40	PHE
3	C	50	MET
3	C	77	GLU
3	C	80	PRO
3	C	113	LEU
3	C	138	TRP
3	C	143	ILE
3	C	165	GLU
3	C	200	LEU
3	C	203	THR
3	C	204	VAL
3	C	215	PHE
3	C	220	VAL
3	C	232	ILE
3	C	239	MET
3	C	244	HIS
3	C	258	ASP
4	D	9	HIS

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Mol	Chain	Res	Type
4	D	16	ILE
4	D	27	ILE
4	D	28	LYS
4	D	41	LEU
4	D	48	ASN
5	H	35	SER
5	H	44	ARG
5	H	57	ARG
5	H	81	LEU
5	H	82	GLN
5	H	89	GLU
5	H	93	MET
5	H	98	ARG
5	H	110	GLN
5	H	115	THR
6	L	2	ILE
6	L	19	VAL
6	L	22	THR
6	L	39	LYS
6	L	42	LYS
6	L	47	LEU
6	L	50	ASN
6	L	53	THR
6	L	67	SER
6	L	71	PHE
6	L	79	LEU
6	L	89	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	HIS
1	A	83	ASN
1	A	113	ASN
1	A	119	HIS
1	A	131	ASN
1	A	132	ASN
1	A	155	ASN
1	A	206	ASN
1	A	269	HIS
1	A	457	ASN
1	A	463	GLN

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Mol	Chain	Res	Type
1	A	469	GLN
1	A	486	ASN
1	A	521	ASN
1	A	541	HIS
2	B	29	HIS
2	B	36	HIS
2	B	65	ASN
2	B	74	ASN
2	B	160	ASN
2	B	173	GLN
2	B	192	GLN
2	B	223	ASN
3	C	6	HIS
3	C	216	HIS
4	D	19	GLN
5	H	39	GLN
6	L	37	GLN
6	L	38	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 3 are monoatomic - leaving 5 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	$\# Z  > 2$
7	HEA	A	602	1	57,67,67	1.43	7 (12%)	61,103,103	1.32	10 (16%)
11	CUA	B	301	2	0,1,1	-	-	-	-	-
7	HEA	A	601	1	57,67,67	1.35	6 (10%)	61,103,103	1.25	7 (11%)
12	PC1	C	301	-	53,53,53	1.52	2 (3%)	59,61,61	1.01	2 (3%)
12	PC1	C	302	-	53,53,53	1.41	3 (5%)	59,61,61	0.88	3 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	PC1	C	302	-	-	10/57/57/57	-
7	HEA	A	601	1	-	9/32/76/76	-
12	PC1	C	301	-	-	17/57/57/57	-
7	HEA	A	602	1	-	11/32/76/76	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	301	PC1	O21-C21	8.10	1.57	1.34
12	C	302	PC1	O31-C31	6.73	1.53	1.33
12	C	301	PC1	O31-C31	6.38	1.52	1.33
12	C	302	PC1	O21-C21	6.36	1.52	1.34
7	A	602	HEA	C3C-CAC	-4.92	1.37	1.47
7	A	602	HEA	C3A-CMA	4.06	1.55	1.46
7	A	601	HEA	C3A-C2A	-3.95	1.34	1.40
7	A	602	HEA	C3C-C2C	-3.95	1.34	1.40
7	A	601	HEA	C3C-CAC	-3.73	1.40	1.47
7	A	601	HEA	C3A-CMA	3.43	1.54	1.46
7	A	602	HEA	C3A-C2A	-3.09	1.36	1.40
12	C	302	PC1	O21-C2	-2.43	1.40	1.46
7	A	601	HEA	C14-C15	2.27	1.38	1.33
7	A	601	HEA	C1C-CHC	-2.23	1.34	1.41
7	A	602	HEA	C22-C23	2.23	1.38	1.32
7	A	602	HEA	C14-C15	2.22	1.38	1.33
7	A	601	HEA	C18-C19	2.09	1.38	1.33
7	A	602	HEA	C18-C19	2.08	1.38	1.33

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	C	301	PC1	C3-C2-C1	-4.71	100.64	111.79
7	A	601	HEA	C17-C18-C19	-2.96	120.53	127.66
7	A	602	HEA	C4B-NB-C1B	-2.76	102.23	105.07
12	C	302	PC1	C11-C12-N	-2.72	106.68	115.78
12	C	301	PC1	C11-C12-N	-2.53	107.33	115.78
12	C	302	PC1	C2-O21-C21	-2.52	111.58	117.79
7	A	602	HEA	C1D-ND-C4D	-2.52	102.47	105.07
7	A	601	HEA	C13-C14-C15	-2.47	121.71	127.66
7	A	602	HEA	C3D-C4D-ND	2.46	112.74	110.36
7	A	601	HEA	C4A-CHB-C1B	2.43	125.77	122.56
7	A	601	HEA	CMC-C2C-C1C	-2.41	124.75	128.46
7	A	602	HEA	O1A-CGA-CBA	-2.36	115.49	123.08
7	A	602	HEA	O2A-CGA-CBA	2.28	121.36	114.03
7	A	602	HEA	C17-C18-C19	-2.28	122.17	127.66
7	A	601	HEA	CMC-C2C-C3C	2.21	128.82	124.68
12	C	302	PC1	C3-O31-C31	-2.21	108.93	117.12
7	A	601	HEA	C4D-CHA-C1A	2.18	125.44	122.56
7	A	602	HEA	C2B-C1B-NB	2.15	112.45	109.88
7	A	602	HEA	O2D-CGD-CBD	2.14	120.89	114.03
7	A	601	HEA	C2B-C1B-NB	2.11	112.41	109.88
7	A	602	HEA	C13-C12-C11	-2.07	111.23	114.35
7	A	602	HEA	C3C-C4C-NC	2.04	111.85	109.21

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	601	HEA	C21-C22-C23-C25
7	A	602	HEA	C18-C19-C20-C21
7	A	602	HEA	C27-C19-C20-C21
7	A	602	HEA	C21-C22-C23-C24
12	C	301	PC1	O22-C21-O21-C2
12	C	301	PC1	C22-C21-O21-C2
12	C	302	PC1	O13-C11-C12-N
7	A	602	HEA	C21-C22-C23-C25
12	C	301	PC1	O32-C31-O31-C3
12	C	301	PC1	C32-C31-O31-C3
12	C	301	PC1	C2A-C2B-C2C-C2D
12	C	302	PC1	C2A-C2B-C2C-C2D
7	A	601	HEA	C21-C22-C23-C24
7	A	602	HEA	C15-C16-C17-C18

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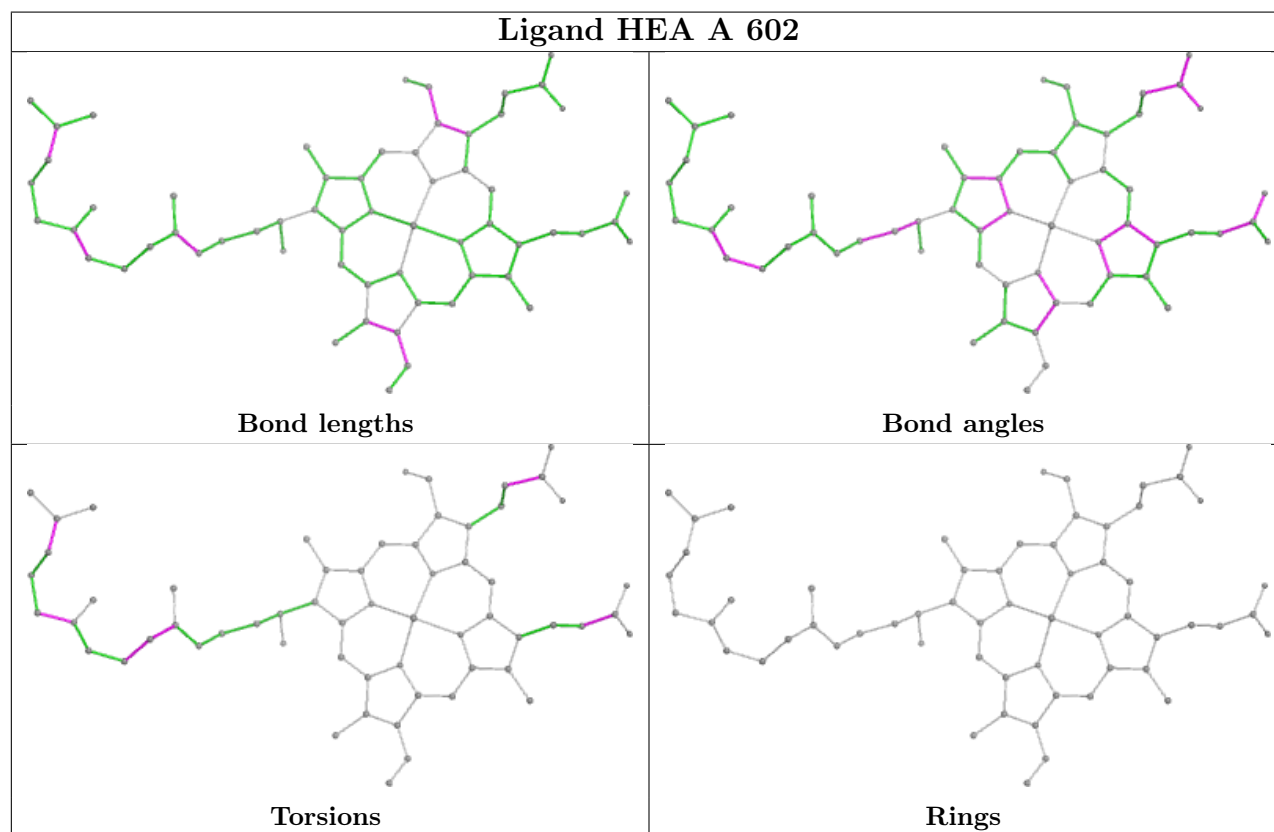
Mol	Chain	Res	Type	Atoms
12	C	301	PC1	C31-C32-C33-C34
12	C	302	PC1	C22-C21-O21-C2
12	C	302	PC1	O22-C21-O21-C2
12	C	301	PC1	C36-C37-C38-C39
12	C	302	PC1	O11-C1-C2-C3
12	C	301	PC1	C21-C22-C23-C24
12	C	302	PC1	O11-C1-C2-O21
7	A	601	HEA	C15-C16-C17-C18
12	C	301	PC1	C34-C35-C36-C37
12	C	301	PC1	C35-C36-C37-C38
12	C	302	PC1	C12-C11-O13-P
12	C	301	PC1	C37-C38-C39-C3A
12	C	301	PC1	C38-C39-C3A-C3B
12	C	301	PC1	C3E-C3F-C3G-C3H
12	C	301	PC1	C33-C34-C35-C36
12	C	302	PC1	C11-O13-P-O11
12	C	302	PC1	C1-O11-P-O13
7	A	601	HEA	C26-C15-C16-C17
7	A	601	HEA	C27-C19-C20-C21
7	A	602	HEA	CAD-CBD-CGD-O1D
12	C	301	PC1	C24-C25-C26-C27
7	A	601	HEA	CAA-CBA-CGA-O2A
7	A	601	HEA	CAA-CBA-CGA-O1A
7	A	601	HEA	C14-C15-C16-C17
12	C	301	PC1	C3D-C3E-C3F-C3G
12	C	301	PC1	C22-C23-C24-C25
7	A	602	HEA	CAD-CBD-CGD-O2D
7	A	602	HEA	C26-C15-C16-C17
7	A	601	HEA	C18-C19-C20-C21
7	A	602	HEA	C14-C15-C16-C17
7	A	602	HEA	CAA-CBA-CGA-O2A
12	C	302	PC1	O21-C21-C22-C23
7	A	602	HEA	CAA-CBA-CGA-O1A

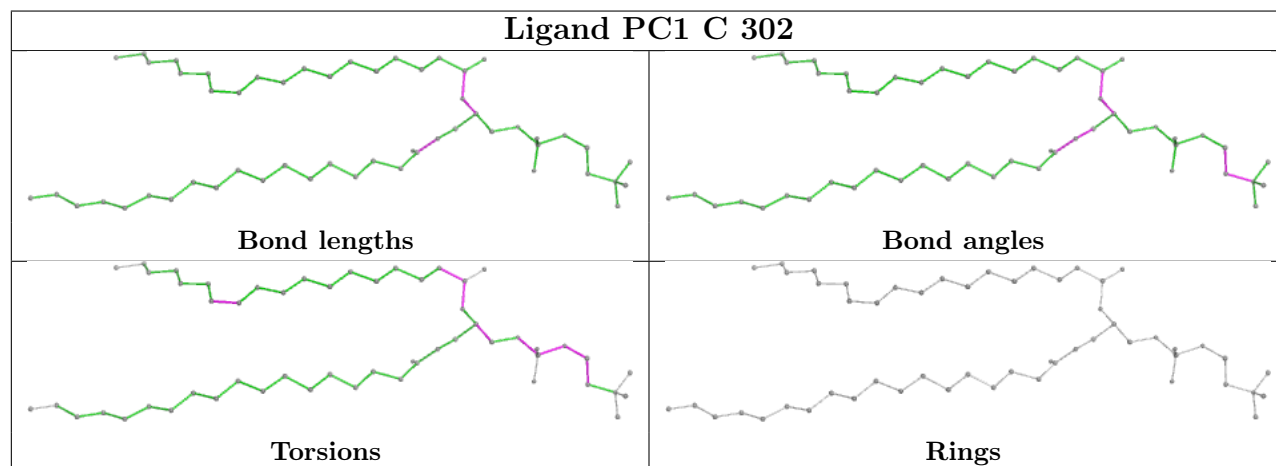
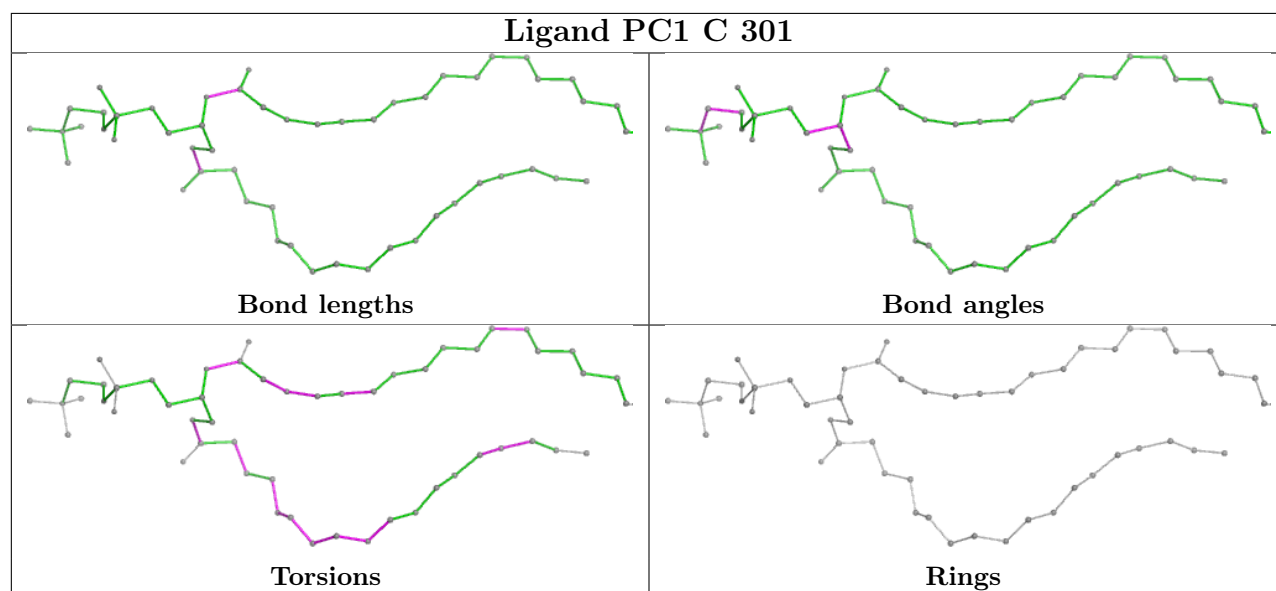
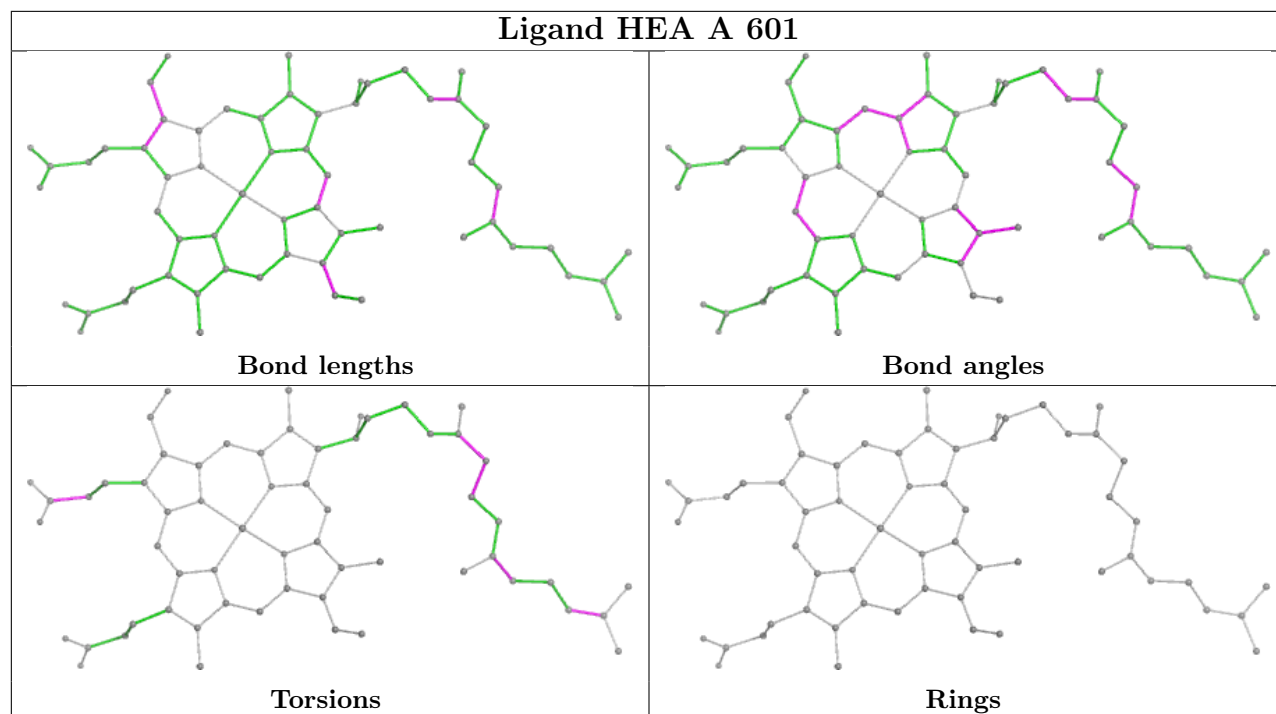
There are no ring outliers.

4 monomers are involved in 58 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	602	HEA	12	0
7	A	601	HEA	20	0
12	C	301	PC1	10	0
12	C	302	PC1	16	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







## 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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.