



Full wwPDB EM Validation Report ⓘ

Mar 19, 2026 – 08:44 PM UTC

PDB ID : 7AU6 / pdb_00007au6
EMDB ID : EMD-11925
Title : Cytochrome c oxidase structure in O-state
Authors : Kolbe, F.; Safarian, S.; Michel, H.
Deposited on : 2020-11-02
Resolution : 2.40 Å(reported)
Based on initial model : 3HB3

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

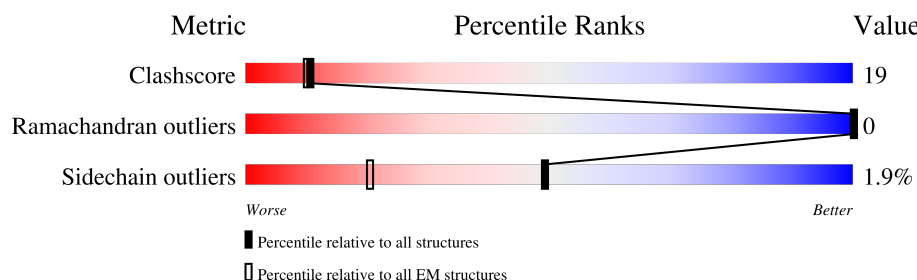
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.40 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)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	558	71% 24% . .
2	B	298	52% 30% . 17%
3	C	274	60% 36% . .
4	D	50	54% 18% . 24%

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
8	OXY	A	609	-	-	X	-

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 9024 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 subunit 1-beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	537	Total	C	N	O	S	0	0
			4257	2854	667	703	33		

- Molecule 2 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	248	Total	C	N	O	S	0	0
			1947	1278	314	347	8		

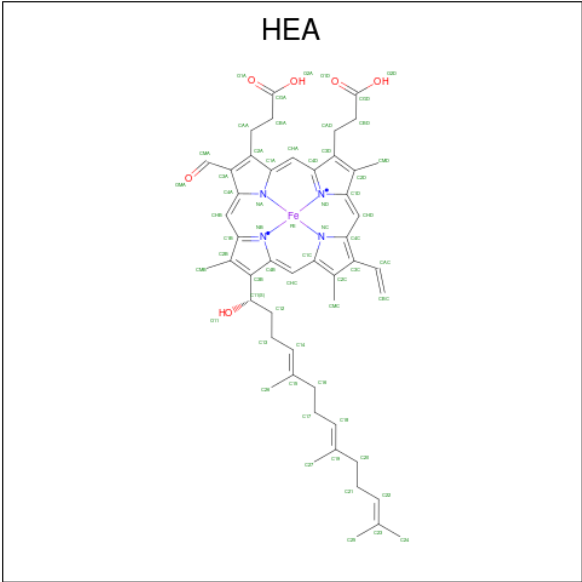
- Molecule 3 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	269	Total	C	N	O	S	0	0
			2150	1463	332	344	11		

- Molecule 4 is a protein called Cytochrome c oxidase subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	38	Total	C	N	O	S	0	0
			288	188	48	51	1		

- Molecule 5 is HEME-A (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 6 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total	Cu	0
			1	1	

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

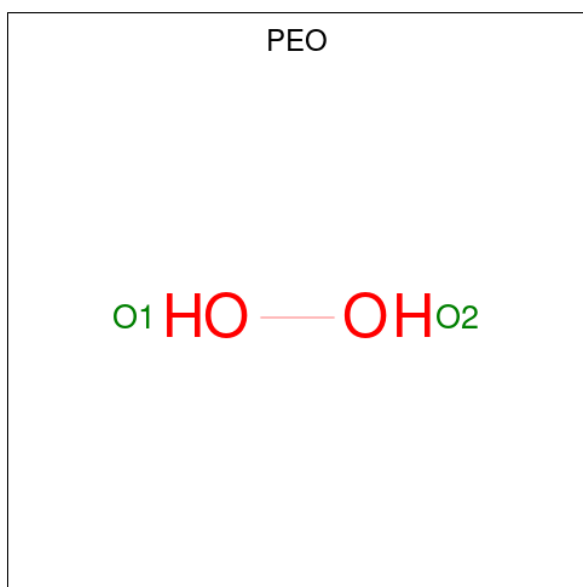
Mol	Chain	Residues	Atoms		AltConf
7	A	1	Total	Ca	0
			1	1	

- Molecule 8 is OXYGEN MOLECULE (CCD ID: OXY) (formula: O₂).



Mol	Chain	Residues	Atoms	AltConf
8	A	1	Total O 2 2	0
8	A	1	Total O 2 2	0
8	A	1	Total O 2 2	0
8	A	1	Total O 2 2	0
8	A	1	Total O 2 2	0
8	A	1	Total O 2 2	0

- Molecule 9 is HYDROGEN PEROXIDE (CCD ID: PEO) (formula: H_2O_2).

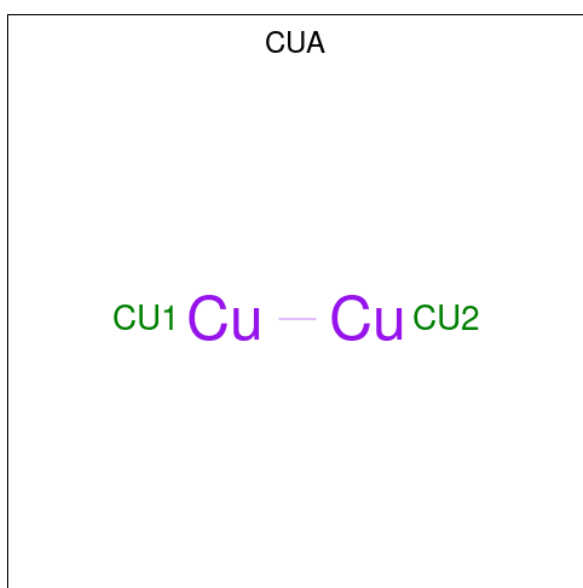


Mol	Chain	Residues	Atoms		AltConf
9	A	1	Total	O	0
			2	2	

- Molecule 10 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

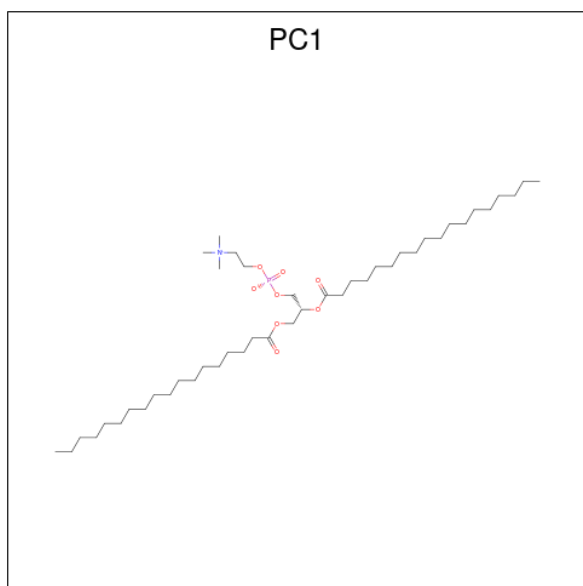
Mol	Chain	Residues	Atoms		AltConf
10	A	1	Total	Mn	0
			1	1	

- Molecule 11 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu₂).



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

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



Mol	Chain	Residues	Atoms					AltConf
12	C	1	Total	C	N	O	P	0
			41	31	1	8	1	
12	C	1	Total	C	N	O	P	0
			54	44	1	8	1	

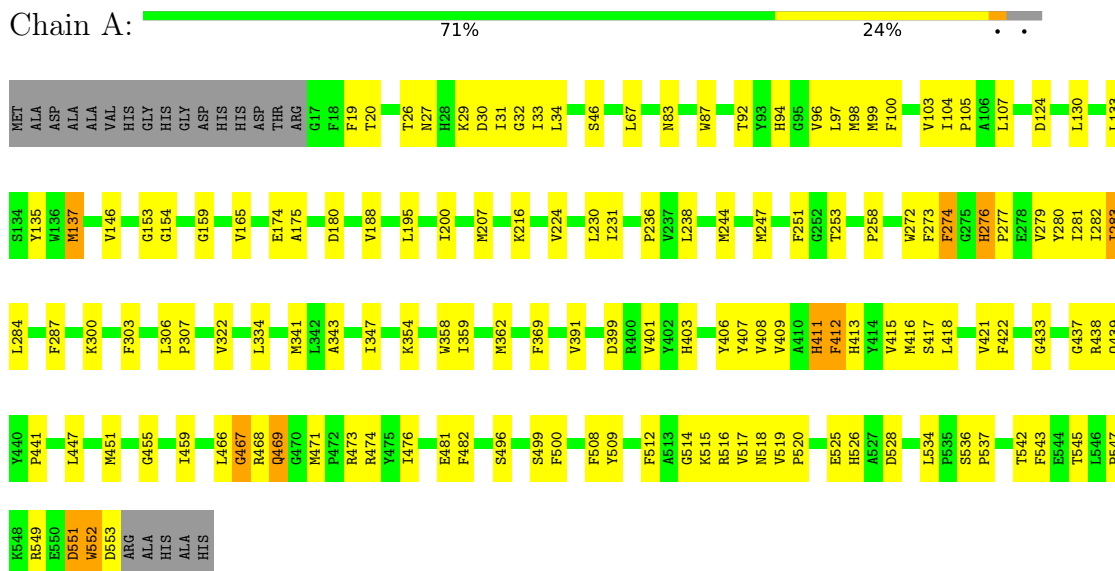
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		AltConf
13	A	98	Total	O	0
			98	98	
13	B	40	Total	O	0
			40	40	
13	C	8	Total	O	0
			8	8	
13	D	2	Total	O	0
			2	2	

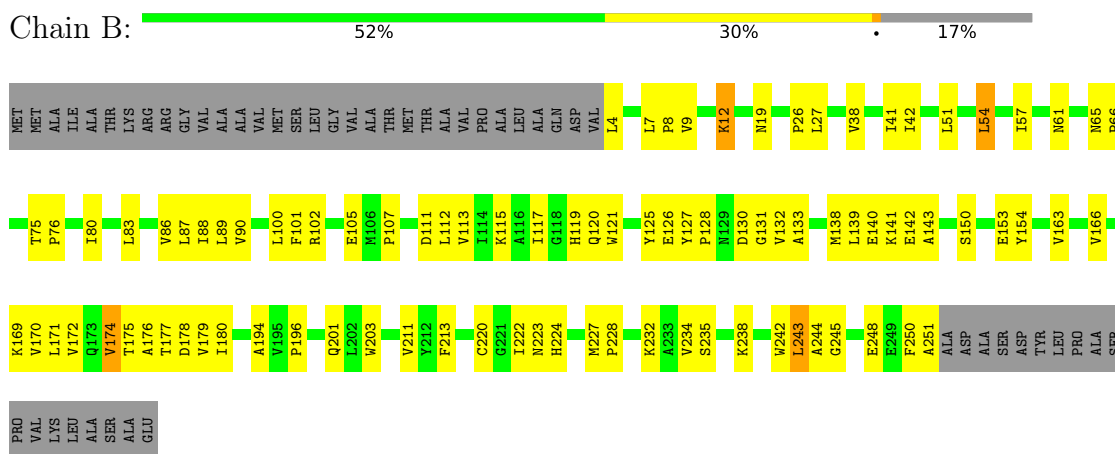
3 Residue-property plots

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.

- Molecule 1: Cytochrome c oxidase subunit 1-beta



- Molecule 2: Cytochrome c oxidase subunit 2



- Molecule 3: Cytochrome c oxidase subunit 3





● Molecule 4: Cytochrome c oxidase subunit 4



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	321273	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor

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: PC1, OXY, CU, CUA, PEO, CA, HEA, MN

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	1.20	28/4416 (0.6%)	1.28	17/6028 (0.3%)
2	B	0.66	10/2004 (0.5%)	0.75	7/2747 (0.3%)
3	C	0.29	0/2235	0.48	2/3060 (0.1%)
4	D	0.76	1/293 (0.3%)	0.87	2/395 (0.5%)
All	All	0.92	39/8948 (0.4%)	1.01	28/12230 (0.2%)

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	31	ILE	C-O	-22.19	0.99	1.24
1	A	34	LEU	C-O	-18.71	1.02	1.24
1	A	33	ILE	C-O	-15.62	1.06	1.24
1	A	33	ILE	N-CA	-14.85	1.28	1.46
1	A	31	ILE	N-CA	-14.69	1.29	1.46
1	A	34	LEU	N-CA	-12.54	1.31	1.46
1	A	135	TYR	C-O	-11.60	1.10	1.24
1	A	273	PHE	C-O	-9.58	1.12	1.24
2	B	179	VAL	C-O	-9.42	1.12	1.23
1	A	34	LEU	CA-C	8.83	1.64	1.52
1	A	32	GLY	C-O	-8.79	1.13	1.23
1	A	469	GLN	C-O	-8.64	1.12	1.24
1	A	32	GLY	N-CA	-8.63	1.34	1.45
2	B	172	VAL	C-O	-8.30	1.15	1.24
1	A	104	ILE	C-O	-8.26	1.17	1.24
1	A	133	LEU	C-O	-8.20	1.14	1.24
4	D	41	LEU	C-O	-7.70	1.15	1.24
1	A	468	ARG	C-O	-6.97	1.15	1.24
2	B	178	ASP	C-O	-6.94	1.15	1.24
2	B	8	PRO	C-O	-6.93	1.16	1.23
1	A	105	PRO	C-O	-6.92	1.15	1.24
1	A	31	ILE	C-N	6.75	1.43	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	180	ILE	C-O	-6.69	1.16	1.24
1	A	34	LEU	CB-CG	-6.67	1.40	1.53
1	A	31	ILE	CA-CB	6.32	1.61	1.54
2	B	171	LEU	C-O	-6.22	1.16	1.24
1	A	272	TRP	C-O	-6.08	1.16	1.24
2	B	170	VAL	C-O	-5.87	1.17	1.24
1	A	33	ILE	CA-C	5.83	1.60	1.52
2	B	175	THR	C-N	-5.78	1.25	1.33
2	B	177	THR	C-O	-5.76	1.16	1.24
1	A	19	PHE	C-O	-5.69	1.17	1.24
2	B	174	VAL	C-N	5.65	1.41	1.33
1	A	97	LEU	C-O	-5.27	1.18	1.24
1	A	236	PRO	C-O	-5.13	1.17	1.24
1	A	411	HIS	C-O	-5.11	1.18	1.24
1	A	552	TRP	C-O	-5.09	1.17	1.24
1	A	20	THR	C-O	-5.09	1.18	1.24
1	A	467	GLY	C-O	-5.04	1.17	1.23

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	276	HIS	CA-CB-CG	-14.78	99.02	113.80
2	B	175	THR	O-C-N	-13.96	104.21	122.78
1	A	30	ASP	CA-C-N	10.46	133.74	120.56
1	A	30	ASP	C-N-CA	10.46	133.74	120.56
1	A	31	ILE	CA-C-O	-8.64	112.01	121.17
2	B	174	VAL	CA-C-N	-8.10	109.49	122.53
2	B	174	VAL	C-N-CA	-8.10	109.49	122.53
4	D	41	LEU	N-CA-C	-8.01	102.55	111.28
2	B	7	LEU	CA-C-N	7.70	127.99	119.90
2	B	7	LEU	C-N-CA	7.70	127.99	119.90
1	A	137	MET	N-CA-C	-7.36	103.28	111.82
1	A	412	PHE	CA-CB-CG	7.28	121.08	113.80
1	A	466	LEU	CA-C-N	6.54	127.19	120.00
1	A	466	LEU	C-N-CA	6.54	127.19	120.00
1	A	369	PHE	CB-CA-C	6.47	121.75	111.91
2	B	175	THR	CA-C-N	6.35	132.77	122.29
2	B	175	THR	C-N-CA	6.35	132.77	122.29
1	A	26	THR	N-CA-C	-6.07	103.97	113.02
1	A	274	PHE	CA-C-N	6.00	126.77	119.99
1	A	274	PHE	C-N-CA	6.00	126.77	119.99
1	A	412	PHE	CB-CA-C	5.92	121.54	110.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	42	GLY	CA-C-N	-5.80	105.15	122.71
3	C	42	GLY	C-N-CA	-5.80	105.15	122.71
1	A	31	ILE	CA-C-N	5.59	126.29	120.03
1	A	31	ILE	C-N-CA	5.59	126.29	120.03
1	A	94	HIS	CA-C-O	-5.38	114.84	120.55
1	A	303	PHE	CA-CB-CG	5.27	119.07	113.80
4	D	46	LEU	N-CA-C	5.23	117.06	111.36

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	4257	0	4171	136	0
2	B	1947	0	1935	76	0
3	C	2150	0	2113	116	0
4	D	288	0	293	18	0
5	A	120	0	107	15	0
6	A	1	0	0	0	0
7	A	1	0	0	0	0
8	A	12	0	0	5	0
9	A	2	0	0	0	0
10	A	1	0	0	0	0
11	B	2	0	0	0	0
12	C	95	0	144	14	0
13	A	98	0	0	40	0
13	B	40	0	0	5	0
13	C	8	0	0	4	0
13	D	2	0	0	0	0
All	All	9024	0	8763	330	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 19.

All (330) 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)
1:A:334:LEU:HD21	2:B:101:PHE:CD1	1.66	1.31
1:A:103:VAL:HB	13:A:782:HOH:O	1.23	1.27
3:C:114:TYR:CE1	12:C:301:PC1:H133	1.78	1.18
1:A:334:LEU:HD21	2:B:101:PHE:CE1	1.81	1.16
3:C:240:THR:HG22	3:C:242:LYS:H	1.12	1.08
1:A:276:HIS:NE2	1:A:280:TYR:HE2	1.57	1.02
5:A:602:HEA:H263	13:A:729:HOH:O	1.61	1.00
12:C:301:PC1:H352	12:C:301:PC1:H251	1.44	0.97
3:C:173:ASN:HA	3:C:176:ILE:HD12	1.46	0.97
1:A:334:LEU:HD21	2:B:101:PHE:HD1	1.29	0.95
1:A:276:HIS:NE2	1:A:280:TYR:CE2	2.32	0.94
1:A:438:ARG:NH1	1:A:514:GLY:O	1.99	0.94
1:A:154:GLY:N	1:A:174:GLU:OE2	2.01	0.92
1:A:334:LEU:CD2	2:B:101:PHE:CE1	2.53	0.91
5:A:602:HEA:H132	13:A:729:HOH:O	1.71	0.91
1:A:153:GLY:C	1:A:174:GLU:OE2	2.16	0.89
1:A:276:HIS:HE2	1:A:280:TYR:HE2	0.91	0.86
3:C:114:TYR:CD1	12:C:301:PC1:H133	2.10	0.86
3:C:58:VAL:HG12	3:C:62:MET:HE2	1.57	0.84
2:B:121:TRP:CG	2:B:223:ASN:HB2	2.12	0.84
3:C:9:GLN:NE2	3:C:77:GLU:OE1	2.11	0.83
1:A:391:VAL:HG23	13:A:729:HOH:O	1.78	0.83
3:C:59:LEU:HD23	3:C:62:MET:CE	2.08	0.83
1:A:124:ASP:HB2	13:A:783:HOH:O	1.79	0.83
1:A:341:MET:HE1	2:B:100:LEU:HD22	1.59	0.82
3:C:240:THR:HG22	3:C:242:LYS:N	1.93	0.82
3:C:172:ILE:HD13	3:C:235:LEU:HG	1.60	0.82
1:A:180:ASP:OD2	3:C:36:LYS:HE3	1.82	0.79
1:A:447:LEU:O	1:A:451:MET:HG3	1.83	0.78
1:A:416:MET:SD	13:A:796:HOH:O	2.42	0.77
1:A:238:LEU:CD1	13:A:787:HOH:O	2.33	0.77
1:A:437:GLY:O	1:A:516:ARG:HD2	1.84	0.76
1:A:334:LEU:CD2	2:B:101:PHE:CD1	2.59	0.76
1:A:153:GLY:CA	1:A:174:GLU:OE2	2.34	0.76
3:C:127:TRP:HB3	3:C:128:PRO:HD3	1.68	0.75
4:D:38:ILE:O	4:D:42:VAL:HG23	1.85	0.74
3:C:70:VAL:O	3:C:74:GLU:HG2	1.86	0.74
2:B:88:ILE:HG22	13:B:440:HOH:O	1.86	0.74
1:A:279:VAL:HG11	8:A:605:OXY:O2	1.88	0.74
3:C:244:HIS:O	3:C:248:GLU:HG3	1.87	0.73
1:A:247:MET:HE2	3:C:211:MET:CE	2.17	0.73
3:C:81:VAL:HG13	4:D:16:ILE:CG2	2.19	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:75:THR:N	2:B:76:PRO:HD2	2.05	0.72
1:A:282:ILE:HG21	13:A:798:HOH:O	1.89	0.72
1:A:46:SER:HB3	1:A:98:MET:HE2	1.71	0.71
1:A:455:GLY:O	1:A:459:ILE:HG13	1.90	0.71
3:C:164:LEU:HD13	3:C:164:LEU:O	1.89	0.71
4:D:45:ALA:HA	4:D:49:SER:OG	1.90	0.71
1:A:230:LEU:HB3	13:A:791:HOH:O	1.90	0.71
1:A:439:GLN:HB3	1:A:515:LYS:HZ3	1.55	0.70
1:A:174:GLU:OE2	1:A:175:ALA:O	2.09	0.70
4:D:42:VAL:O	4:D:46:LEU:HD13	1.91	0.70
3:C:176:ILE:HG22	3:C:180:ILE:HD11	1.73	0.70
2:B:132:VAL:HA	2:B:250:PHE:O	1.92	0.70
3:C:81:VAL:HG13	4:D:16:ILE:HG21	1.72	0.70
1:A:391:VAL:HG13	13:A:794:HOH:O	1.91	0.69
3:C:144:ASN:ND2	3:C:188:LEU:HB3	2.10	0.67
1:A:174:GLU:CD	1:A:175:ALA:O	2.36	0.67
3:C:136:ASP:OD1	3:C:138:TRP:N	2.23	0.66
1:A:238:LEU:HD12	13:A:787:HOH:O	1.93	0.66
3:C:149:LEU:O	3:C:153:VAL:HG23	1.94	0.66
1:A:551:ASP:OD1	1:A:551:ASP:N	2.27	0.66
3:C:227:LEU:HD12	3:C:250:ALA:HB1	1.78	0.65
1:A:334:LEU:CD2	2:B:101:PHE:HE1	2.07	0.65
1:A:180:ASP:OD2	3:C:36:LYS:CE	2.43	0.65
1:A:354:LYS:HD3	13:A:793:HOH:O	1.97	0.65
3:C:172:ILE:HG23	3:C:231:LEU:CD1	2.27	0.65
2:B:141:LYS:HG2	2:B:154:TYR:CD1	2.33	0.64
3:C:87:GLN:HA	3:C:90:PHE:CE2	2.33	0.64
1:A:98:MET:HB3	5:A:601:HEA:CAC	2.28	0.64
3:C:80:PRO:HB2	4:D:16:ILE:HD13	1.80	0.63
1:A:153:GLY:HA2	1:A:174:GLU:OE2	1.98	0.63
3:C:230:CYS:O	3:C:234:LEU:HD12	1.99	0.63
1:A:247:MET:HE2	3:C:211:MET:HE1	1.79	0.62
3:C:216:HIS:CE1	3:C:261:TRP:HB2	2.34	0.62
3:C:59:LEU:HD23	3:C:62:MET:HE3	1.80	0.62
3:C:144:ASN:OD1	3:C:185:PHE:HA	2.00	0.62
3:C:93:PHE:O	3:C:97:GLU:HG2	2.00	0.61
2:B:140:GLU:O	2:B:143:ALA:N	2.32	0.61
2:B:4:LEU:HD22	2:B:234:VAL:HG11	1.82	0.61
3:C:127:TRP:CZ2	3:C:205:TYR:HD2	2.18	0.60
1:A:408:VAL:HB	13:A:702:HOH:O	2.02	0.60
3:C:168:ARG:NH2	3:C:234:LEU:HA	2.17	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:543:PHE:CD1	1:A:547:PRO:HG3	2.37	0.59
3:C:240:THR:CG2	3:C:242:LYS:H	2.00	0.59
3:C:176:ILE:O	3:C:180:ILE:HD12	2.02	0.59
5:A:602:HEA:HBC1	5:A:602:HEA:HMC3	1.82	0.59
1:A:276:HIS:CD2	1:A:276:HIS:C	2.81	0.59
3:C:86:LEU:HD13	12:C:302:PC1:O22	2.01	0.59
12:C:301:PC1:H352	12:C:301:PC1:C25	2.27	0.59
2:B:166:VAL:HG22	2:B:234:VAL:O	2.02	0.59
1:A:277:PRO:HB3	13:A:791:HOH:O	2.03	0.58
1:A:238:LEU:HD13	13:A:787:HOH:O	1.97	0.58
3:C:127:TRP:CB	3:C:128:PRO:HD3	2.34	0.58
1:A:418:LEU:C	13:A:703:HOH:O	2.45	0.58
3:C:163:VAL:HG23	3:C:164:LEU:H	1.68	0.58
2:B:245:GLY:O	2:B:248:GLU:HG2	2.04	0.58
3:C:160:HIS:HA	3:C:163:VAL:CG2	2.34	0.58
3:C:228:PHE:O	3:C:232:ILE:HG12	2.03	0.58
1:A:276:HIS:CE1	1:A:280:TYR:HE2	2.20	0.57
3:C:159:HIS:O	3:C:163:VAL:HG22	2.04	0.57
2:B:138:MET:HG3	2:B:228:PRO:CD	2.34	0.57
3:C:115:PRO:HD2	3:C:124:ASP:HB3	1.86	0.57
1:A:282:ILE:HD12	13:A:796:HOH:O	2.05	0.56
3:C:45:VAL:HG11	3:C:50:MET:CE	2.36	0.56
3:C:134:THR:HG22	3:C:205:TYR:CZ	2.40	0.56
2:B:130:ASP:O	2:B:132:VAL:HG23	2.05	0.56
3:C:115:PRO:HG3	3:C:127:TRP:HA	1.87	0.56
3:C:136:ASP:OD1	3:C:136:ASP:C	2.49	0.56
3:C:175:LEU:HD21	3:C:247:PHE:CE1	2.41	0.56
1:A:473:ARG:CD	13:A:702:HOH:O	2.54	0.56
3:C:164:LEU:HD12	3:C:165:GLU:OE2	2.06	0.56
1:A:515:LYS:O	1:A:515:LYS:HG3	2.05	0.55
2:B:126:GLU:O	2:B:128:PRO:HD3	2.05	0.55
3:C:45:VAL:HG11	3:C:50:MET:HE3	1.87	0.55
3:C:115:PRO:CG	3:C:127:TRP:HA	2.37	0.55
3:C:160:HIS:HA	3:C:163:VAL:HG22	1.89	0.55
2:B:139:LEU:HD22	2:B:143:ALA:HB1	1.89	0.55
1:A:334:LEU:CG	2:B:101:PHE:CE1	2.90	0.55
1:A:27:ASN:HD21	1:A:29:LYS:HB2	1.72	0.55
2:B:86:VAL:O	2:B:90:VAL:HG23	2.05	0.55
1:A:516:ARG:NH2	1:A:518:ASN:OD1	2.40	0.55
2:B:111:ASP:HB2	2:B:169:LYS:O	2.07	0.54
1:A:276:HIS:CE1	1:A:280:TYR:CE2	2.94	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:TRP:HZ3	13:A:797:HOH:O	1.90	0.54
3:C:172:ILE:HG22	3:C:176:ILE:HD11	1.90	0.54
1:A:231:ILE:HG13	1:A:281:ILE:HG12	1.89	0.54
4:D:36:LEU:O	4:D:40:VAL:HG23	2.08	0.54
1:A:200:ILE:HG21	1:A:224:VAL:HG12	1.90	0.53
1:A:216:LYS:HE3	1:A:549:ARG:HH21	1.72	0.53
1:A:341:MET:CE	2:B:100:LEU:HD22	2.34	0.53
3:C:222:ILE:HD13	12:C:302:PC1:H3C2	1.89	0.53
3:C:40:PHE:O	3:C:41:PHE:HB2	2.08	0.53
1:A:247:MET:HE2	3:C:211:MET:HE3	1.89	0.53
1:A:276:HIS:O	1:A:279:VAL:HG22	2.08	0.53
3:C:137:PRO:HD3	3:C:273:ARG:HD3	1.91	0.53
1:A:471:MET:HB2	1:A:482:PHE:CE1	2.44	0.53
13:A:794:HOH:O	2:B:89:LEU:HD22	2.09	0.53
3:C:139:HIS:O	3:C:142:LEU:N	2.42	0.52
2:B:220:CYS:SG	2:B:224:HIS:HA	2.49	0.52
1:A:253:THR:HA	13:C:404:HOH:O	2.08	0.52
1:A:359:ILE:HA	1:A:362:MET:HE2	1.91	0.52
1:A:422:PHE:HD1	13:A:703:HOH:O	1.94	0.51
3:C:141:PRO:O	3:C:145:THR:OG1	2.26	0.51
2:B:101:PHE:O	2:B:105:GLU:HG3	2.11	0.51
3:C:135:PHE:HZ	3:C:196:ALA:CB	2.24	0.51
3:C:200:LEU:O	3:C:201:ALA:HB3	2.09	0.51
5:A:602:HEA:C13	13:A:729:HOH:O	2.44	0.51
2:B:121:TRP:HA	2:B:227:MET:SD	2.50	0.50
1:A:549:ARG:HG2	1:A:553:ASP:HB3	1.93	0.50
1:A:417:SER:O	1:A:421:VAL:HB	2.11	0.50
1:A:500:PHE:HB2	5:A:601:HEA:H261	1.92	0.50
2:B:57:ILE:O	2:B:61:ASN:ND2	2.32	0.50
1:A:334:LEU:HD11	2:B:101:PHE:CD1	2.46	0.50
1:A:67:LEU:HA	1:A:83:ASN:HB2	1.94	0.50
2:B:9:VAL:CG1	2:B:12:LYS:HE2	2.41	0.50
3:C:59:LEU:HD23	3:C:62:MET:HE1	1.93	0.50
3:C:81:VAL:HG22	13:C:407:HOH:O	2.12	0.49
1:A:549:ARG:HG3	1:A:552:TRP:CZ2	2.47	0.49
1:A:137:MET:HE3	1:A:188:VAL:HG13	1.94	0.49
2:B:9:VAL:HG11	2:B:12:LYS:HE2	1.93	0.49
2:B:201:GLN:HB2	13:B:414:HOH:O	2.13	0.49
2:B:211:VAL:HG22	2:B:232:LYS:HG2	1.95	0.49
3:C:168:ARG:NH2	3:C:237:GLY:HA2	2.28	0.49
1:A:401:VAL:HA	13:A:790:HOH:O	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:LEU:HB3	1:A:307:PRO:HD3	1.95	0.49
3:C:144:ASN:HD21	3:C:188:LEU:HB3	1.77	0.49
3:C:33:ALA:HA	3:C:38:ILE:HG23	1.95	0.49
3:C:8:TYR:CE2	4:D:14:MET:HE1	2.48	0.48
3:C:114:TYR:CD1	12:C:301:PC1:C13	2.90	0.48
1:A:473:ARG:NH1	13:A:702:HOH:O	2.36	0.48
1:A:415:VAL:HG11	13:A:795:HOH:O	2.13	0.48
3:C:172:ILE:O	3:C:176:ILE:HG13	2.13	0.48
1:A:27:ASN:HA	13:A:713:HOH:O	2.14	0.48
1:A:87:TRP:HB2	1:A:476:ILE:HG13	1.95	0.48
2:B:26:PRO:HB3	2:B:102:ARG:HH12	1.77	0.48
2:B:112:LEU:HD12	2:B:113:VAL:H	1.78	0.48
3:C:135:PHE:HZ	3:C:196:ALA:HB2	1.79	0.48
2:B:121:TRP:CD1	2:B:223:ASN:HB2	2.49	0.47
3:C:189:GLN:OE1	3:C:189:GLN:HA	2.14	0.47
1:A:545:THR:HA	3:C:5:ASN:HB3	1.96	0.47
2:B:238:LYS:HB3	2:B:238:LYS:HZ2	1.79	0.47
1:A:406:TYR:CE1	1:A:471:MET:HE2	2.50	0.47
1:A:92:THR:O	1:A:96:VAL:HG23	2.15	0.47
1:A:258:PRO:HG2	2:B:196:PRO:HB2	1.95	0.47
3:C:59:LEU:HA	3:C:62:MET:HE3	1.96	0.47
3:C:193:TYR:OH	3:C:213:THR:OG1	2.13	0.47
1:A:481:GLU:OE2	2:B:12:LYS:HD3	2.14	0.47
2:B:150:SER:N	2:B:153:GLU:OE2	2.32	0.47
3:C:172:ILE:CD1	3:C:235:LEU:HG	2.39	0.47
3:C:176:ILE:HG22	3:C:180:ILE:CD1	2.43	0.47
3:C:127:TRP:CD2	3:C:127:TRP:C	2.91	0.47
12:C:301:PC1:H292	4:D:41:LEU:HD11	1.97	0.47
2:B:119:HIS:O	2:B:121:TRP:N	2.48	0.47
1:A:99:MET:SD	1:A:416:MET:HE1	2.55	0.47
1:A:549:ARG:HG3	1:A:552:TRP:CH2	2.50	0.47
2:B:87:LEU:HD23	2:B:87:LEU:N	2.29	0.46
3:C:127:TRP:CE3	3:C:127:TRP:O	2.68	0.46
3:C:244:HIS:CD2	3:C:248:GLU:HG2	2.49	0.46
2:B:75:THR:N	2:B:76:PRO:CD	2.77	0.46
3:C:81:VAL:HG13	4:D:16:ILE:HG22	1.94	0.46
3:C:129:PRO:HB2	3:C:203:THR:HG21	1.97	0.46
1:A:525:GLU:HG2	1:A:526:HIS:N	2.31	0.46
5:A:601:HEA:HBC2	13:A:798:HOH:O	2.15	0.46
1:A:107:LEU:HD12	13:A:782:HOH:O	2.15	0.46
5:A:601:HEA:C4C	13:A:773:HOH:O	2.64	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:602:HEA:H241	13:B:440:HOH:O	2.14	0.46
2:B:27:LEU:HD22	13:B:429:HOH:O	2.16	0.46
3:C:39:THR:HG23	3:C:42:GLY:C	2.40	0.46
2:B:150:SER:OG	2:B:153:GLU:OE2	2.34	0.46
2:B:174:VAL:CG1	2:B:194:ALA:HB2	2.46	0.46
2:B:243:LEU:O	2:B:244:ALA:C	2.57	0.46
2:B:138:MET:HG3	2:B:228:PRO:CG	2.46	0.46
2:B:140:GLU:O	2:B:141:LYS:C	2.58	0.46
3:C:66:TRP:CG	12:C:302:PC1:H332	2.51	0.45
4:D:45:ALA:O	4:D:49:SER:OG	2.34	0.45
2:B:9:VAL:HG13	2:B:213:PHE:HE2	1.81	0.45
1:A:441:PRO:HG3	1:A:509:TYR:CE1	2.51	0.45
3:C:172:ILE:HG23	3:C:231:LEU:HD13	1.98	0.45
3:C:18:PHE:CZ	3:C:22:ILE:HD11	2.51	0.45
3:C:132:ILE:HD13	3:C:132:ILE:HA	1.86	0.45
1:A:284:LEU:HD22	13:A:789:HOH:O	2.16	0.45
1:A:474:ARG:O	2:B:224:HIS:HD2	1.99	0.45
2:B:113:VAL:O	2:B:128:PRO:HD2	2.16	0.45
1:A:469:GLN:NE2	2:B:19:ASN:O	2.33	0.45
1:A:516:ARG:HH12	1:A:518:ASN:HA	1.81	0.45
13:A:794:HOH:O	2:B:89:LEU:CD2	2.64	0.45
3:C:34:TRP:CE2	3:C:48:PRO:HB3	2.51	0.45
3:C:201:ALA:HA	13:C:404:HOH:O	2.16	0.45
1:A:244:MET:HG2	3:C:104:TRP:CZ3	2.52	0.45
4:D:16:ILE:HG13	4:D:20:GLN:OE1	2.17	0.45
3:C:168:ARG:HH21	3:C:234:LEU:HA	1.82	0.45
3:C:230:CYS:SG	3:C:247:PHE:HA	2.56	0.45
3:C:231:LEU:HD12	3:C:231:LEU:O	2.17	0.45
4:D:46:LEU:N	4:D:46:LEU:HD12	2.32	0.44
1:A:287:PHE:CE2	13:A:793:HOH:O	2.57	0.44
1:A:300:LYS:HB3	1:A:300:LYS:HE2	1.53	0.44
2:B:176:ALA:O	2:B:196:PRO:HA	2.16	0.44
1:A:406:TYR:O	1:A:409:VAL:HB	2.17	0.44
3:C:163:VAL:HG23	3:C:164:LEU:N	2.30	0.44
3:C:70:VAL:HG22	12:C:302:PC1:H32	2.00	0.44
1:A:207:MET:HE3	3:C:8:TYR:CD1	2.53	0.44
5:A:602:HEA:HAC	13:A:796:HOH:O	2.17	0.44
2:B:51:LEU:HD23	2:B:51:LEU:HA	1.84	0.44
1:A:416:MET:SD	5:A:602:HEA:HAC	2.58	0.44
1:A:517:VAL:HG23	1:A:517:VAL:O	2.18	0.44
3:C:81:VAL:CG1	4:D:16:ILE:HG22	2.47	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:MET:HE1	13:A:796:HOH:O	2.18	0.44
2:B:125:TYR:O	2:B:133:ALA:HA	2.18	0.44
3:C:266:VAL:HG23	3:C:267:VAL:HG23	2.00	0.44
1:A:433:GLY:HA2	1:A:438:ARG:O	2.18	0.43
3:C:135:PHE:CZ	3:C:196:ALA:HA	2.53	0.43
2:B:235:SER:OG	2:B:238:LYS:HG3	2.18	0.43
3:C:137:PRO:HG2	3:C:138:TRP:CE2	2.53	0.43
1:A:473:ARG:HD2	13:A:702:HOH:O	2.17	0.43
3:C:80:PRO:HD2	13:C:407:HOH:O	2.18	0.43
1:A:543:PHE:CE1	1:A:547:PRO:HG3	2.53	0.43
2:B:131:GLY:O	2:B:251:ALA:HA	2.18	0.43
3:C:113:LEU:HD13	3:C:271:TRP:CH2	2.53	0.43
1:A:67:LEU:CA	1:A:83:ASN:HB2	2.49	0.43
1:A:130:LEU:HD11	1:A:195:LEU:HD22	2.00	0.43
2:B:115:LYS:HG2	2:B:117:ILE:HD11	2.00	0.43
1:A:96:VAL:HG22	8:A:609:OXY:O1	2.18	0.43
4:D:41:LEU:HA	4:D:41:LEU:HD23	1.67	0.43
1:A:334:LEU:HG	2:B:101:PHE:CE1	2.54	0.43
1:A:549:ARG:HA	1:A:552:TRP:NE1	2.34	0.43
3:C:83:ARG:HD3	3:C:243:GLN:HG3	2.01	0.43
3:C:115:PRO:HG2	3:C:125:GLY:O	2.19	0.43
5:A:601:HEA:HBC1	5:A:601:HEA:CMC	2.49	0.42
1:A:549:ARG:HA	1:A:552:TRP:CE2	2.54	0.42
12:C:302:PC1:H2I3	12:C:302:PC1:H3C1	2.00	0.42
2:B:121:TRP:CZ2	2:B:222:ILE:HG22	2.55	0.42
1:A:508:PHE:O	1:A:512:PHE:HD1	2.02	0.42
2:B:245:GLY:O	2:B:248:GLU:CG	2.65	0.42
4:D:45:ALA:CA	4:D:49:SER:OG	2.64	0.42
1:A:411:HIS:O	1:A:415:VAL:HG22	2.20	0.42
5:A:602:HEA:H122	13:A:795:HOH:O	2.19	0.42
1:A:280:TYR:HA	1:A:283:ILE:HG22	2.00	0.42
2:B:120:GLN:C	2:B:121:TRP:CG	2.97	0.42
3:C:127:TRP:CB	3:C:128:PRO:CD	2.97	0.42
3:C:139:HIS:O	3:C:140:LEU:C	2.63	0.42
1:A:238:LEU:HB2	1:A:274:PHE:CG	2.54	0.42
3:C:175:LEU:HD21	3:C:247:PHE:HE1	1.82	0.42
1:A:96:VAL:HG11	8:A:606:OXY:O1	2.19	0.42
1:A:418:LEU:CA	13:A:703:HOH:O	2.68	0.42
1:A:528:ASP:OD1	1:A:528:ASP:N	2.48	0.42
1:A:165:VAL:HA	8:A:610:OXY:O1	2.19	0.42
1:A:407:TYR:HB2	1:A:467:GLY:HA3	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:54:LEU:HD13	2:B:54:LEU:HA	1.72	0.42
2:B:88:ILE:CG2	13:B:440:HOH:O	2.57	0.42
3:C:262:LEU:O	3:C:266:VAL:HG13	2.19	0.42
1:A:409:VAL:HG13	1:A:413:HIS:CE1	2.55	0.41
3:C:239:MET:HA	12:C:302:PC1:H142	2.01	0.41
1:A:341:MET:HE2	1:A:341:MET:HB2	1.82	0.41
1:A:496:SER:O	1:A:499:SER:OG	2.31	0.41
5:A:602:HEA:HBC1	5:A:602:HEA:CMC	2.47	0.41
1:A:399:ASP:OD2	1:A:403:HIS:HB2	2.21	0.41
2:B:41:ILE:HG21	2:B:88:ILE:HG23	2.02	0.41
3:C:175:LEU:CD1	3:C:234:LEU:HD13	2.50	0.41
1:A:100:PHE:CE2	8:A:609:OXY:O2	2.74	0.41
1:A:247:MET:HE3	1:A:251:PHE:HB2	2.02	0.41
2:B:121:TRP:CD2	2:B:223:ASN:HB2	2.53	0.41
3:C:243:GLN:O	12:C:302:PC1:H143	2.20	0.41
3:C:45:VAL:CG1	3:C:50:MET:HE3	2.49	0.41
1:A:153:GLY:HA3	1:A:159:GLY:O	2.21	0.41
2:B:142:GLU:CD	2:B:142:GLU:H	2.28	0.41
3:C:62:MET:HB3	3:C:66:TRP:CZ3	2.56	0.41
3:C:137:PRO:HB3	3:C:269:TYR:HB3	2.01	0.41
1:A:282:ILE:HD13	13:A:798:HOH:O	2.21	0.41
2:B:163:VAL:HG21	2:B:242:TRP:CE2	2.56	0.41
4:D:46:LEU:N	4:D:46:LEU:CD1	2.84	0.41
1:A:98:MET:HB3	5:A:601:HEA:HAC	2.00	0.41
1:A:276:HIS:HB3	1:A:277:PRO:HD3	2.02	0.41
1:A:322:VAL:HG12	1:A:343:ALA:HB1	2.02	0.41
1:A:536:SER:HA	1:A:537:PRO:HA	1.91	0.41
2:B:174:VAL:HG12	2:B:194:ALA:HB2	2.03	0.41
2:B:107:PRO:HD3	2:B:203:TRP:CG	2.56	0.41
3:C:99:MET:HE1	12:C:301:PC1:H2B2	2.02	0.41
1:A:230:LEU:CB	13:A:791:HOH:O	2.61	0.40
1:A:409:VAL:HA	1:A:412:PHE:CE2	2.56	0.40
1:A:473:ARG:HD3	13:A:702:HOH:O	2.20	0.40
1:A:516:ARG:NH1	1:A:518:ASN:HA	2.36	0.40
1:A:520:PRO:HA	1:A:534:LEU:O	2.22	0.40
1:A:471:MET:HB2	1:A:482:PHE:CD1	2.56	0.40
2:B:65:ASN:O	2:B:66:PRO:C	2.62	0.40
1:A:549:ARG:HG2	1:A:553:ASP:CB	2.51	0.40
2:B:38:VAL:O	2:B:42:ILE:HG12	2.21	0.40
3:C:8:TYR:CZ	4:D:14:MET:HE1	2.56	0.40
3:C:142:LEU:HD12	3:C:142:LEU:HA	1.78	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:127:TYR:HB2	2:B:132:VAL:HB	2.03	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 PDB entries followed by that with respect to all EM entries.

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	174/558 (31%)	165 (95%)	9 (5%)	0	100	100
2	B	231/298 (78%)	222 (96%)	9 (4%)	0	100	100
3	C	267/274 (97%)	256 (96%)	11 (4%)	0	100	100
4	D	36/50 (72%)	35 (97%)	1 (3%)	0	100	100
All	All	708/1180 (60%)	678 (96%)	30 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	440/454 (97%)	434 (99%)	6 (1%)	59	79
2	B	208/243 (86%)	203 (98%)	5 (2%)	43	65
3	C	217/221 (98%)	211 (97%)	6 (3%)	38	60
4	D	29/40 (72%)	29 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	894/958 (93%)	877 (98%)	17 (2%)	49 71

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	146	VAL
1	A	283	ILE
1	A	347	ILE
1	A	519	VAL
1	A	542	THR
1	A	551	ASP
2	B	12	LYS
2	B	54	LEU
2	B	80	ILE
2	B	83	LEU
2	B	243	LEU
3	C	75	THR
3	C	81	VAL
3	C	155	VAL
3	C	172	ILE
3	C	188	LEU
3	C	231	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	113	ASN
1	A	155	ASN
2	B	104	GLN
2	B	215	GLN
3	C	9	GLN
3	C	159	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 3 are monoatomic - leaving 12 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
8	OXY	A	608	-	1,1,1	0.40	0	-		
8	OXY	A	610	-	1,1,1	0.23	0	-		
8	OXY	A	609	-	1,1,1	0.27	0	-		
5	HEA	A	602	1,9	67,67,67	2.03	14 (20%)	81,103,103	2.10	25 (30%)
8	OXY	A	605	-	1,1,1	0.27	0	-		
11	CUA	B	301	2	0,1,1	-	-	-		
8	OXY	A	607	-	1,1,1	0.29	0	-		
12	PC1	C	302	-	53,53,53	0.38	0	59,61,61	0.63	2 (3%)
8	OXY	A	606	-	1,1,1	0.26	0	-		
9	PEO	A	611	6,5	1,1,1	0.03	0	-		
5	HEA	A	601	1	67,67,67	2.22	17 (25%)	81,103,103	2.66	34 (41%)
12	PC1	C	301	-	40,40,53	1.30	3 (7%)	46,48,61	3.01	17 (36%)

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
5	HEA	A	602	1,9	-	12/36/76/76	-
12	PC1	C	302	-	-	19/57/57/57	-
5	HEA	A	601	1	-	12/36/76/76	-
12	PC1	C	301	-	-	19/44/44/57	-

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	601	HEA	FE-NB	7.46	2.17	1.94
5	A	602	HEA	FE-NB	7.10	2.16	1.94
5	A	602	HEA	FE-NA	6.50	2.16	1.95
5	A	601	HEA	FE-ND	6.35	2.14	1.94
5	A	601	HEA	FE-NC	5.94	2.14	1.95
5	A	602	HEA	FE-ND	5.44	2.11	1.94
5	A	601	HEA	C4A-NA	-5.36	1.29	1.39
5	A	601	HEA	C1B-NB	-5.12	1.28	1.38
5	A	602	HEA	C1D-ND	-4.78	1.32	1.40
5	A	601	HEA	C4B-NB	-4.60	1.32	1.40
12	C	301	PC1	O21-C2	-4.42	1.36	1.46
12	C	301	PC1	O31-C31	4.20	1.45	1.33
5	A	602	HEA	C4D-ND	-4.05	1.30	1.38
5	A	601	HEA	C4D-ND	-4.03	1.30	1.38
5	A	602	HEA	C1A-NA	-3.94	1.32	1.39
5	A	602	HEA	C4A-NA	-3.46	1.33	1.39
5	A	602	HEA	FE-NC	3.09	2.05	1.95
5	A	601	HEA	FE-NA	2.89	2.04	1.95
5	A	602	HEA	C11-C3B	2.73	1.54	1.51
5	A	601	HEA	CHD-C4C	-2.72	1.33	1.39
5	A	601	HEA	C1D-ND	-2.60	1.35	1.40
5	A	602	HEA	C4B-NB	-2.56	1.35	1.40
5	A	601	HEA	C1C-NC	-2.49	1.34	1.39
5	A	601	HEA	C1B-C2B	-2.39	1.39	1.44
5	A	602	HEA	CAC-C3C	2.28	1.53	1.47
5	A	602	HEA	O2A-CGA	-2.26	1.23	1.30
12	C	301	PC1	O22-C21	-2.23	1.15	1.22
5	A	602	HEA	CMA-C3A	2.21	1.50	1.45
5	A	601	HEA	C1A-NA	-2.18	1.35	1.39
5	A	601	HEA	C3C-C2C	-2.12	1.34	1.41
5	A	601	HEA	O2D-CGD	-2.11	1.23	1.30
5	A	602	HEA	C3C-C2C	-2.09	1.34	1.41
5	A	601	HEA	C3D-C2D	-2.06	1.32	1.36
5	A	601	HEA	CMB-C2B	2.04	1.55	1.50

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	601	HEA	C4B-NB-C1B	8.93	115.78	105.21
12	C	301	PC1	C15-N-C13	-8.47	86.73	108.98
12	C	301	PC1	O21-C2-C1	-8.23	78.82	108.34
12	C	301	PC1	C15-N-C14	-7.57	89.09	108.98
5	A	601	HEA	C4A-NA-C1A	7.10	117.40	105.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	601	HEA	C2A-C1A-NA	-6.78	103.78	110.32
12	C	301	PC1	O21-C21-C22	6.66	125.89	111.48
5	A	602	HEA	C1D-ND-C4D	6.44	112.83	105.21
5	A	601	HEA	C12-C11-C3B	6.39	122.11	112.12
5	A	601	HEA	C3B-C4B-NB	-6.27	102.64	109.84
12	C	301	PC1	O21-C21-O22	-5.98	109.72	123.70
5	A	602	HEA	C4B-NB-C1B	4.93	111.05	105.21
12	C	301	PC1	C14-N-C13	4.78	121.53	108.98
5	A	602	HEA	CAD-CBD-CGD	-4.65	101.32	113.67
5	A	602	HEA	C4A-NA-C1A	4.61	113.33	105.82
5	A	602	HEA	C2A-C1A-NA	-4.40	106.08	110.32
5	A	601	HEA	CHB-C4A-C3A	4.34	132.53	125.21
5	A	601	HEA	C4A-CHB-C1B	4.33	135.23	126.02
5	A	601	HEA	C4A-C3A-C2A	4.20	110.46	106.81
5	A	602	HEA	C1A-CHA-C4D	3.97	134.45	126.02
5	A	602	HEA	CAA-CBA-CGA	-3.77	103.67	113.67
12	C	301	PC1	C34-C33-C32	-3.76	99.31	113.13
12	C	301	PC1	C3-O31-C31	3.69	130.60	117.12
5	A	601	HEA	O11-C11-C12	3.64	118.80	109.14
5	A	602	HEA	C3D-C4D-ND	-3.62	106.85	110.35
5	A	602	HEA	C3C-C4C-NC	-3.54	106.82	109.80
5	A	601	HEA	C2B-C1B-NB	-3.50	105.86	109.90
5	A	601	HEA	CHC-C4B-C3B	3.43	134.47	125.80
5	A	601	HEA	OMA-CMA-C3A	-3.42	117.91	125.62
5	A	601	HEA	C24-C23-C22	-3.28	112.82	122.66
5	A	602	HEA	C3B-C4B-NB	-3.24	106.12	109.84
5	A	602	HEA	C2D-C1D-ND	-3.16	106.20	109.84
5	A	601	HEA	CHB-C1B-C2B	3.03	129.82	125.03
12	C	301	PC1	O21-C2-C3	3.01	119.13	108.34
5	A	601	HEA	C13-C14-C15	-2.99	120.77	127.62
5	A	601	HEA	C13-C12-C11	-2.95	109.68	114.39
5	A	602	HEA	CHC-C1C-NC	2.95	129.21	123.86
5	A	601	HEA	CMB-C2B-C1B	-2.93	120.46	125.03
5	A	602	HEA	C24-C23-C22	-2.88	114.00	122.66
5	A	601	HEA	C3C-C4C-NC	-2.86	107.39	109.80
5	A	601	HEA	C17-C16-C15	2.84	122.58	113.19
5	A	601	HEA	C1D-ND-C4D	2.82	108.55	105.21
12	C	301	PC1	C15-N-C12	-2.82	98.72	109.91
5	A	601	HEA	CAA-CBA-CGA	-2.78	106.28	113.67
5	A	601	HEA	C1C-CHC-C4B	2.75	132.70	126.25
5	A	602	HEA	C2B-C1B-NB	-2.73	106.75	109.90
12	C	301	PC1	C11-C12-N	-2.73	107.06	115.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	602	HEA	CHA-C1A-C2A	2.66	129.07	124.86
5	A	601	HEA	C21-C22-C23	-2.61	118.92	127.64
5	A	601	HEA	CHA-C1A-NA	2.61	127.30	124.45
5	A	602	HEA	O2A-CGA-O1A	-2.57	116.72	123.33
12	C	301	PC1	C36-C35-C34	-2.56	101.42	114.37
5	A	602	HEA	CHA-C4D-C3D	2.54	128.48	124.77
5	A	601	HEA	CMC-C2C-C1C	-2.52	121.58	125.42
5	A	601	HEA	CHA-C1A-C2A	2.52	128.85	124.86
5	A	601	HEA	O11-C11-C3B	-2.47	106.73	111.26
5	A	601	HEA	CHD-C1D-ND	2.46	127.41	124.37
5	A	602	HEA	C17-C18-C19	-2.45	122.02	127.62
12	C	301	PC1	C33-C32-C31	-2.43	104.78	113.69
12	C	302	PC1	O21-C21-O22	-2.42	118.04	123.70
5	A	602	HEA	C4C-NC-C1C	2.39	109.72	105.82
12	C	302	PC1	O21-C21-C22	2.39	116.64	111.48
5	A	602	HEA	CAD-C3D-C4D	-2.38	120.56	124.70
12	C	301	PC1	C13-N-C12	2.35	119.25	109.91
12	C	301	PC1	C23-C22-C21	-2.30	105.25	113.69
12	C	301	PC1	C14-N-C12	2.29	119.03	109.91
5	A	601	HEA	CHC-C1C-NC	2.23	127.90	123.86
5	A	601	HEA	O2D-CGD-O1D	-2.21	117.64	123.33
5	A	602	HEA	CAD-C3D-C2D	2.15	131.89	127.87
5	A	602	HEA	CMC-C2C-C1C	-2.14	122.16	125.42
5	A	601	HEA	C12-C13-C14	2.13	117.76	112.16
5	A	602	HEA	CHB-C4A-C3A	2.12	128.78	125.21
5	A	601	HEA	C26-C15-C14	-2.10	118.25	123.63
5	A	601	HEA	O2A-CGA-CBA	2.09	120.61	114.00
5	A	601	HEA	CBD-CAD-C3D	-2.07	106.81	112.53
5	A	602	HEA	CBD-CAD-C3D	2.07	118.24	112.53
12	C	301	PC1	C35-C34-C33	-2.02	104.15	114.37
5	A	602	HEA	CMB-C2B-C3B	-2.02	126.37	130.28

There are no chirality outliers.

All (62) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	601	HEA	C2A-C3A-CMA-OMA
5	A	601	HEA	C4A-C3A-CMA-OMA
5	A	602	HEA	C2A-C3A-CMA-OMA
12	C	301	PC1	C1-O11-P-O14
12	C	301	PC1	C12-C11-O13-P
12	C	301	PC1	O13-C11-C12-N

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
12	C	301	PC1	O22-C21-O21-C2
12	C	301	PC1	C22-C21-O21-C2
12	C	302	PC1	C11-O13-P-O11
12	C	302	PC1	O13-C11-C12-N
12	C	302	PC1	O11-C1-C2-O21
12	C	302	PC1	O22-C21-O21-C2
12	C	302	PC1	C22-C21-O21-C2
12	C	302	PC1	O32-C31-O31-C3
12	C	302	PC1	C32-C31-O31-C3
5	A	601	HEA	C21-C22-C23-C24
12	C	301	PC1	C11-C12-N-C14
5	A	601	HEA	C15-C16-C17-C18
5	A	602	HEA	C2D-C3D-CAD-CBD
12	C	301	PC1	C11-C12-N-C15
12	C	302	PC1	C35-C36-C37-C38
12	C	302	PC1	C25-C26-C27-C28
12	C	302	PC1	C24-C25-C26-C27
12	C	301	PC1	C23-C24-C25-C26
5	A	602	HEA	C4D-C3D-CAD-CBD
12	C	301	PC1	C32-C33-C34-C35
5	A	601	HEA	C17-C18-C19-C27
12	C	302	PC1	C28-C29-C2A-C2B
12	C	301	PC1	C2-C1-O11-P
12	C	302	PC1	C36-C37-C38-C39
5	A	601	HEA	C26-C15-C16-C17
12	C	301	PC1	C22-C23-C24-C25
5	A	602	HEA	C27-C19-C20-C21
12	C	302	PC1	O11-C1-C2-C3
12	C	302	PC1	C29-C2A-C2B-C2C
12	C	301	PC1	C26-C27-C28-C29
5	A	602	HEA	C21-C22-C23-C24
12	C	301	PC1	C24-C25-C26-C27
12	C	302	PC1	C23-C24-C25-C26
12	C	302	PC1	C34-C35-C36-C37
12	C	301	PC1	C27-C28-C29-C2A
5	A	602	HEA	C4A-C3A-CMA-OMA
12	C	301	PC1	O21-C2-C3-O31
12	C	302	PC1	C11-O13-P-O14
5	A	601	HEA	C14-C15-C16-C17
5	A	602	HEA	C19-C20-C21-C22
12	C	301	PC1	C38-C39-C3A-C3B
5	A	601	HEA	C21-C22-C23-C25

Continued on next page...

Continued from previous page...

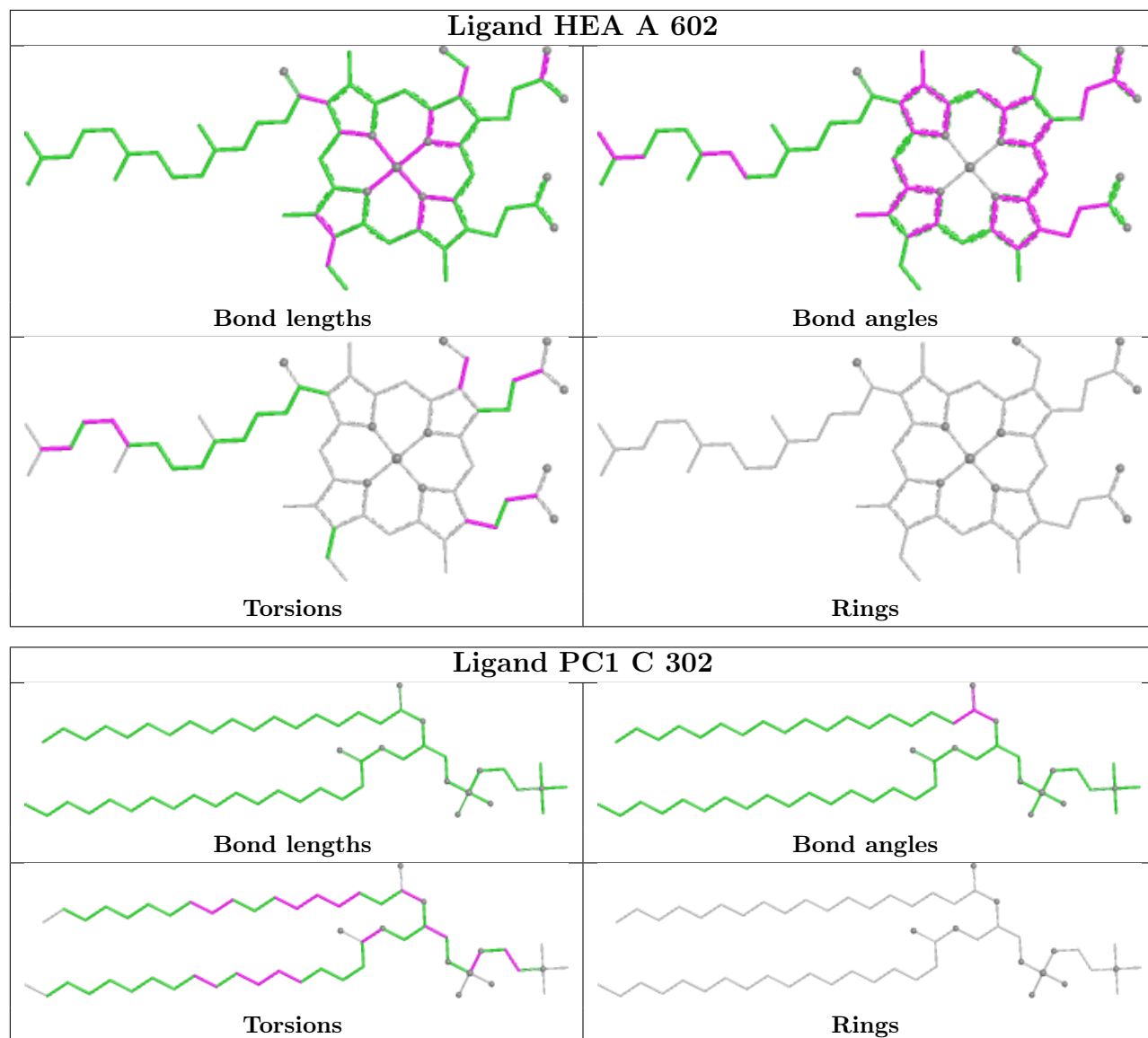
Mol	Chain	Res	Type	Atoms
5	A	601	HEA	C18-C19-C20-C21
12	C	302	PC1	C38-C39-C3A-C3B
12	C	301	PC1	C1-C2-O21-C21
5	A	602	HEA	CAD-CBD-CGD-O2D
5	A	602	HEA	CAA-CBA-CGA-O1A
12	C	301	PC1	C34-C35-C36-C37
5	A	602	HEA	C18-C19-C20-C21
12	C	302	PC1	C22-C23-C24-C25
5	A	602	HEA	CAD-CBD-CGD-O1D
5	A	602	HEA	CAA-CBA-CGA-O2A
5	A	601	HEA	CAA-CBA-CGA-O1A
5	A	601	HEA	CAD-CBD-CGD-O1D
12	C	301	PC1	C11-C12-N-C13
5	A	601	HEA	CAA-CBA-CGA-O2A

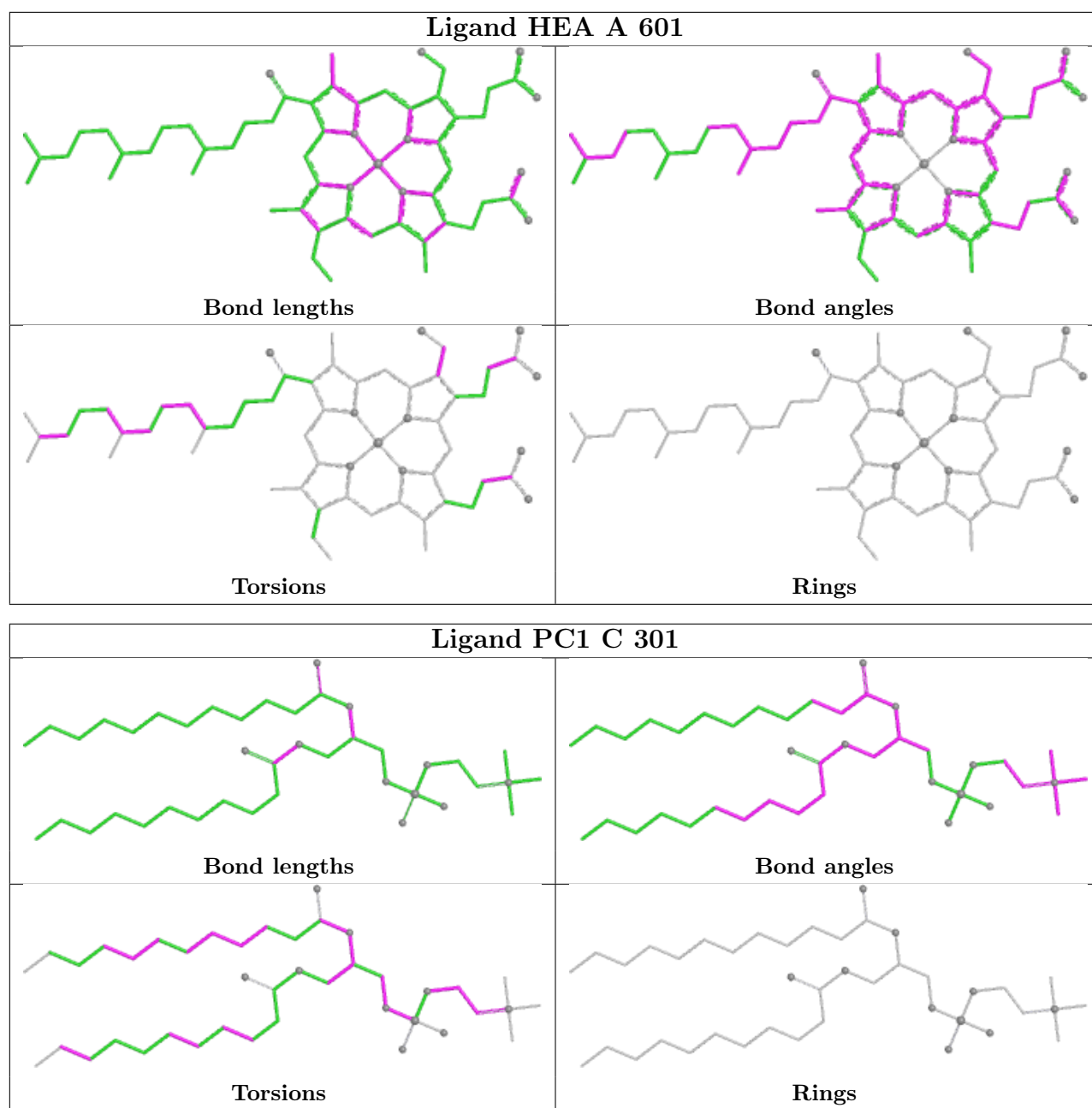
There are no ring outliers.

8 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	610	OXY	1	0
8	A	609	OXY	2	0
5	A	602	HEA	9	0
8	A	605	OXY	1	0
12	C	302	PC1	7	0
8	A	606	OXY	1	0
5	A	601	HEA	6	0
12	C	301	PC1	7	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 Map visualisation

This section contains visualisations of the EMDB entry EMD-11925. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis ⓘ

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.